

Systems Research Institute
Polish Academy of Sciences

**Control and Optimum Design of Distributed
Parameter Systems. Gradient Flow and
Applications to Elasticity Systems**

PhD dissertation

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Warszawa, 2025

Abstract

This dissertation presents a comprehensive study of optimal control and shape optimization problems in elastic systems, combining rigorous theoretical developments with efficient numerical methods. The study covers a range of topics including linear and nonlinear elasticity, boundary contact problems, and control-driven structural design, aiming to build a unified framework that connects analysis with computation.

The study begins with the formulation of the optimal boundary control problem in linear elasticity, where the traction force is considered as the control variable. The problem is transformed into a system of state equations, adjoint equations, and optimality conditions by minimizing a cost function that includes displacement tracking and control energy. The dynamic control problem can be approximated by its static counterpart using the Turnpike property, which asserts that the optimal trajectory tends to a steady-state solution in the long term, significantly reducing the computational burden.

For shape and topology optimization, this dissertation uses shape derivative analysis combined with velocity field methods to guide the structural evolution. The gradient flow formulation transforms the optimization process into a system of time-dependent partial differential equations, which enhances numerical stability and convergence analysis. The method is shown to be very effective in flexibility minimization, shape reconstruction, and inverse problems, outperforming the classical level set method in terms of interpretability, theoretical rigor, and algorithmic control.

In this study, a discontinuous Galerkin (DG) method is used to solve the level set evolution equations when dealing with nonlinear elastic problems. The DG framework enables accurate and robust simulation of the optimization process, thus facilitating effective optimization under challenging mechanical conditions. Numerical experiments confirm the practical applicability of the proposed method.

The contact problem is solved by two approaches. The first approach uses phase field regularization to continuously model the contact interface, enabling sensitivity analysis and smooth structural evolution. The second approach uses topological derivatives to evaluate the impact of internal domain perturbations, especially in regions far from the contact boundary, combined with a phase field approach for optimization. Together, these methods form a flexible and powerful contact-aware shape and topology optimization toolkit.

The shape optimization problem is further analyzed using a gradient flow formulation in the context of a static contact problem, where elastic energy and Kohn Vogelius

Functionals are used as shape functions. Although the associated Hessian matrix is only directional due to non-smoothness, the tapered derivative framework provides a viable foundation. Numerical results show that the gradient flow system exhibits stable convergence despite theoretical challenges.

In summary, this dissertation provides a unified perspective for the control and optimization of elastic systems. It not only contributes important theoretical insights into shape sensitivity, gradient flow, and control mechanisms, but also provides robust and efficient numerical schemes. These findings lay the foundation for future dynamic optimization, multi-physics coupling, and further exploration of Turnpike phenomena in elastic systems.

Key words: Shape optimization, Optimal control, Topological derivative, Gradient flow, Phase field method

Streszczenie

Niniejsza rozprawa przedstawia kompleksowe badanie zagadnień sterowania optymalnego oraz optymalizacji kształtu w układach sprężystych, łącząc rygorystyczne podejście teoretyczne z efektywnymi metodami numerycznymi. Praca obejmuje szeroki zakres zagadnień, w tym elastyczność liniową i nieliniową, problemy kontaktowe na brzegu oraz projektowanie konstrukcyjne oparte na sterowaniu, dążąc do stworzenia zunifikowanego podejścia łączącego analizę z obliczeniami.

Badanie rozpoczyna się od sformułowania problemu optymalnego sterowania brzegowego w elastyczności liniowej, gdzie siła naprężenia jest traktowana jako zmienna sterująca. Problem ten przekształca się w układ równań stanu, równań sprzężonych oraz warunków optymalności poprzez minimalizację funkcjonu kosztu obejmującego śledzenie przemieszczenia i energię sterowania. Problem dynamicznego sterowania można przybliżyć jego statycznym odpowiednikiem za pomocą własności Turnpike, która wskazuje, że trajektoria optymalna dąży do rozwiązania stacjonarnego w dłuższym czasie, co znacznie zmniejsza koszty obliczeniowe.

W kontekście optymalizacji kształtu i topologii, rozprawa ta wykorzystuje analizę pochodnej kształtu w połączeniu z metodami pola prędkości do kierowania ewolucją struktury. Ujęcie w postaci przepływu gradientowego przekształca proces optymalizacji w układ czasowo-zależnych równań różniczkowych cząstkowych, co zwiększa stabilność numeryczną i ułatwia analizę zbieżności. Metoda ta okazała się bardzo skuteczna w minimalizacji podatności, rekonstrukcji kształtu oraz w problemach odwrotnych, przewyższając klasyczną metodę zbioru poziomicowego pod względem interpretowalności, rygoru teoretycznego i kontroli algorytmicznej.

W niniejszym badaniu zastosowano metodę Galerkina nieciągłą (DG) do rozwiązywania równań ewolucji zbioru poziomicowego w przypadku problemów elastyczności nieliniowej. Ramy DG umożliwiają dokładną i odporną symulację procesu optymalizacji, co pozwala na skuteczne rozwiązywanie problemów w wymagających warunkach mechanicznych. Eksperymenty numeryczne potwierdzają praktyczną przydatność proponowanej metody.

Problem kontaktu rozwiązano na dwa sposoby. Pierwsze podejście

wykorzystuje regularizację pola fazowego do ciągłego modelowania interfejsu kontaktowego, co umożliwia analizę wrażliwości i płynną ewolucję struktury. Drugie podejście wykorzystuje pochodne topologiczne do oceny wpływu zaburzeń wewnętrznych w obszarach oddalonych od granicy kontaktu, w połączeniu z podejściem pola fazowego do optymalizacji. Razem metody te tworzą elastyczny i skuteczny zestaw narzędzi do optymalizacji kształtu i topologii uwzględniający kontakt.

Problem optymalizacji kształtu analizowany jest również przy użyciu sformułowania przepływu gradientowego w kontekście statycznego problemu kontaktowego, gdzie energia sprężysta oraz funkcjonały Kohna-Vogeliusa pełnią rolę funkcji kształtu. Choć związana macierz Hessego jest tylko kierunkowa z powodu nieskładalności, ramy pochodnej stępionej stanowią realną podstawę teoretyczną. Wyniki numeryczne pokazują, że układ przepływu gradientowego wykazuje stabilną zbieżność pomimo wyzwań teoretycznych.

Podsumowując, niniejsza rozprawa dostarcza zunifikowanego spojrzenia na sterowanie i optymalizację układów sprężystych. Wnosi istotny wkład teoretyczny w analizę wrażliwości kształtu, przepływu gradientowego i mechanizmów sterowania oraz proponuje solidne i wydajne schematy numeryczne. Wyniki te stanowią podstawę dla przyszłej optymalizacji dynamicznej, sprzężenia wielu fizyk oraz dalszej eksploracji zjawisk Turnpike w układach sprężystych.

Słowa kluczowe: optymalizacja kształtu, sterowanie optymalne, pochodna topologiczna, przepływ gradientowy, metoda pola fazowego

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Chapter 1

Introduction

Elastic systems play a central role in numerous engineering and scientific applications, ranging from structural design and mechanical systems to aerospace engineering. Within this context, the optimal control of elastic behavior and the optimization of structural configurations are fundamental problems that directly impact performance, efficiency, and reliability. However, the inherent complexity of elastic systems—especially in the presence of nonlinear behavior, contact phenomena, and intricate geometries—poses significant challenges to both mathematical modeling and computational analysis.

In recent years, considerable efforts have been devoted to the development of mathematical models and numerical methods for optimal control and structural optimization in elasticity Lewiński et al., 2004. While classical approaches have achieved success in specific settings, limitations remain in addressing large deformations, nonlinear material behavior, and problems with moving or free boundaries. Moreover, bridging the gap between theoretical rigor and practical applicability continues to be an active area of research.

This dissertation presents a comprehensive study of optimal control problems in elastic systems, aiming to develop a rigorous mathematical framework and propose efficient numerical methods for shape and topology optimization. The research encompasses a wide spectrum of models, including linear and nonlinear elasticity, boundary control problems with contact conditions, and engineering-driven design optimization. The overarching goal is to balance theoretical depth with engineering adaptability, providing both analytical insight and computational tools for complex structural design.

The first major contribution of this work lies in the formulation of an optimal control model for linear elastic systems, where boundary traction is employed as the

control variable. By minimizing a cost functional that combines displacement error with control energy, the model guides the system toward a desired target configuration. The problem is solved as a coupled system involving the state equation, adjoint equation, and optimality conditions, thereby establishing a closed-loop relationship between the objective function and the control strategy. Secondly, by exploiting the turnpike property—where the optimal trajectory approximates a steady state over sufficiently long time intervals—time-dependent problems can be simplified to static formulations, thereby significantly enhancing computational efficiency.

In the domain of shape optimization, this work applies shape derivative theory and the velocity field approach to perform sensitivity analysis of the objective functional. A gradient flow-based dynamical system is then constructed, transforming the optimization process into the solution of an evolutionary partial differential equation. This method offers strong numerical stability and theoretical interpretability, making it well-suited to applications such as structural reconstruction and inverse problems. Compared to classical level-set approaches, the proposed method exhibits notable advantages in convergence analysis, controllability, and implementation, offering a more intuitive and practical alternative for shape optimization.

For nonlinear elasticity, the discontinuous Galerkin (DG) method is introduced to handle optimization problems involving highly nonlinear structural behavior and large deformations. As a high-accuracy and flexible discretization technique, the DG method is well-adapted to solving complex variational problems. Extensive numerical experiments demonstrate its superior performance in both nonlinear structural analysis and optimal design, highlighting its strong potential for engineering applications.

Furthermore, the study addresses elastic systems involving contact boundaries by proposing two optimization strategies. The first employs phase-field regularization to smooth the objective functional, enabling the accurate tracking of contact region evolution and supporting shape sensitivity analysis. The second leverages topology derivative theory to assess the impact of microstructural changes away from the contact interface on overall system performance. These strategies can be used independently or in combination, forming a flexible and comprehensive optimization toolbox for structures operating under contact constraints.

In summary, this dissertation presents an in-depth investigation into the optimal control and structural optimization of elastic systems. It contributes to the development of a systematic mathematical theory and demonstrates strong adaptability and practical value in numerical computation and engineering applications. The findings

lay a solid foundation for future research in dynamic optimization, nonlinear coupling mechanisms, and further exploration of the turnpike phenomenon.

1.1 Motivation

With the rapid development of modern engineering and technology, structural design is facing increasingly stringent requirements. Structures must not only meet classical mechanical criteria such as stiffness, strength, and stability, but also exhibit high adaptability, controllability, and efficiency under complex boundary conditions and multi-functional performance goals. This has driven growing attention toward structure–control coupled optimization from both academia and industry.

In elastic systems, structural performance is not solely determined by external loads, but is also strongly influenced by shape, material distribution, and topological features. Especially in applications involving boundary control, unilateral contact conditions, and topological reconfiguration, the geometry of the structure becomes an integral part of the control problem. It acts as a dynamic variable that affects not only mechanical response but also the feasibility and efficiency of control strategies.

While optimal control theory provides a systematic foundation for designing boundary loads and distributed actuation, traditional approaches usually assume a fixed geometry and ignore shape-related sensitivity. As a result, they fall short in applications where structural geometry is actively optimized or where shape evolves during the design process. Conversely, classical shape and topology optimization methods rarely account for the interaction between control inputs and structural adaptation, thereby overlooking a critical coupling that is essential in many engineering scenarios.

Moreover, when contact phenomena—such as friction, unilateral constraints, or adhesion—are present, the resulting variational models often involve non-smooth and non-differentiable functionals. These features make classical gradient-based sensitivity analysis difficult to apply, particularly when dealing with inequality constraints at the boundary. Overcoming these challenges calls for the development of new mathematical formulations, such as phase-field regularization and variational inequality-based modeling, which can capture contact behavior within optimization frameworks.

Additionally, nonlinear elasticity is frequently encountered in high-performance structural applications, such as aerospace, biomechanics, and soft robotics. These systems experience large deformations and strong material nonlinearities, which render linear models insufficient. However, nonlinear elasticity introduces significant com-

plexity: the governing PDEs become highly nonlinear, sensitivity analysis is more involved, and numerical discretization requires advanced techniques such as discontinuous Galerkin methods. This increases the computational burden and limits the applicability of classical design methods.

Given these challenges, there is a strong need for a unified computational framework that can simultaneously handle:

- boundary control optimization;
- shape and topology evolution;
- contact mechanics (including inequality and friction conditions);
- nonlinear elastic behavior.

This dissertation explores several numerical approaches for the control and optimization of elastic structures under complex conditions. Using tools such as shape calculus, topological derivatives, phase-field modeling, and gradient-based methods, the work focuses on representative problems involving geometry, material distribution, contact, and nonlinear effects.

1.2 Main idea

This dissertation systematically studies coupled optimization problems in elastic structures, covering boundary control, shape evolution, topological sensitivity, and interface modeling, with the overall goal of improving structural performance under prescribed functional and mechanical criteria.

The study first constructs an optimal boundary control problem in the context of linear elastic mechanics, where the boundary traction is regarded as a control variable. A cost function is constructed to jointly penalize the deviation from the desired displacement field and the control energy. Through the variational principle, a coupled system consisting of the state equation, the adjoint equation, and the first-order optimal condition is derived. This provides a rigorous theoretical basis for the analysis and implementation of boundary control in elastic structures.

To go beyond fixed geometry control, the framework introduces shape derivative analysis, which enables the evaluation of the sensitivity of the objective function to boundary deformation. This points the way to shape evolution based on variational evolution. As a complement, topological derivatives are used to evaluate the impact of

infinitesimal inclusions or voids within the material domain, allowing the optimization framework to operate across multiple scales. The integration of shape and topological sensitivity helps to achieve a flexible and unified structural adaptation method.

To guide the optimization in a stable and theoretically consistent way, a gradient flow-based dynamic system is introduced. This reformulates the design process as a continuous evolution of a virtual time variable, driven by the shape gradient of the objective function. This formulation not only ensures monotonic energy dissipation, but also a smooth trajectory towards the optimal configuration, which enhances robustness and numerical interpretability compared to traditional update schemes.

This study addresses the inherent non-smoothness of the relevant variational inequalities when dealing with contact mechanics (especially non-penetration and friction constraints). Regularization techniques are introduced to approximate the non-differentiable contact energy using smooth penalty functions, which enables the derivation of differentiable states and adjoint systems. In terms of specific implementation, the phase field method is used to model the internal interface and contact zone in a continuous and implicit manner. The phase field variable can naturally capture the interface evolution while supporting topological derivative-based optimization, providing a powerful tool for contact-aware design.

For nonlinear elastic systems characterized by large deformations and material nonlinearity, the discontinuous Galerkin (DG) method is used to numerically discretize the level set-based evolution equations. This high-order, mesh-flexible method has excellent stability and accuracy, and is particularly suitable for capturing complex mechanical behaviors. The DG framework works well when combined with level sets, enabling accurate control and geometric adaptation even under challenging nonlinear conditions.

In summary, this study develops a unified approach for control, geometry, topology, and interface modeling within a variational optimization framework. It combines theoretical rigor with numerical efficiency, opening up new avenues for the design of smart structures in complex elastic environments.

1.3 Outline and main results

This dissertation is organized into five core chapters, each addressing a key aspect of optimal control and structural optimization in elastic systems. The study integrates concepts from PDE-constrained optimization, variational inequalities, shape and topol-

ogy sensitivity, contact mechanics, and numerical discretization methods. The main contributions of each chapter are summarized as follows:

The chapter 2 establishes the theoretical foundation for optimal boundary control in linear elastic structures. The control variable is the boundary traction, and the objective functional combines displacement tracking with control energy penalization. Variational techniques are employed to derive the first-order optimality system, which consists of the state equation, the adjoint equation, and optimality conditions. Special attention is given to frictional contact boundary scenarios modeled via variational inequalities. The approach is extended through the use of topological derivatives and level set-based shape evolution, enabling simultaneous control and structural design. A preliminary discussion on toll-road characteristics demonstrates that, under suitable assumptions, the dynamic control problem can be approximated by its steady-state counterpart.

The chapter 3 focuses on unilateral contact problems and applies a phase-field method to regularize the inherently nonsmooth contact conditions in Signorini-type problems. A variational inequality formulation is introduced, and the phase-field regularization leads to a continuous contact energy functional. This method facilitates sensitivity analysis and is particularly well-suited for shape and topology optimization. A coupled optimization framework combining phase-field modeling and topological derivatives is proposed, allowing for simultaneous geometric and topological evolution of structures. Frictional contact phenomena are also considered, and corresponding numerical examples are presented. The numerical case studies provided in this chapter demonstrate the effectiveness of the approach in practical contact-driven design.

The chapter 4 introduces a gradient flow framework, modeling shape evolution as a dynamic process driven by the descent direction of a shape functional. This approach transforms shape optimization into a time-dependent PDE system, offering a rigorous and stable evolution path. In static elastic contact problems, shape functionals based on elastic energy or the Kohn-Vogelius criterion are differentiated with respect to the domain using cone or directional derivatives. The convergence of the resulting flows is analyzed numerically, and several related gradient flow examples are provided.

To address the challenges of large deformations and material nonlinearities, the chapter 5 investigates optimal shape design in nonlinear elastic systems. The Discontinuous Galerkin (DG) method is adopted for its high accuracy and flexibility in handling complex geometries. The DG framework is combined with the level set method for boundary evolution, enabling efficient resolution of the evolution equations. Numerical

results validate the robustness of the proposed method in high-strain scenarios.

1.4 Principal notations

$\Omega \subset \mathbb{R}^d$	a bounded open domain in $\mathbb{R}^d$ ($d = 2$, or 3).
$\mathbf{u}$	Displacement field.
$\boldsymbol{\varepsilon}(\mathbf{u})$	Strain tensor.
$\mathbf{g}$	Boundary traction (control variable).
$\mathcal{T}(x)$	Topological derivative.
$C^k(\Omega)$	Space of functions that are k -times continuously differentiable on the closure $\bar{\Omega}$, with $k \in \mathbb{N}_0$.
$\mathcal{D}(\Omega)$	Space of infinitely differentiable functions with compact support in Ω ; equipped with the inductive limit topology (test function space).
$\mathcal{D}'(\Omega)$	Dual space of $\mathcal{D}(\Omega)$, i.e., the space of distributions on Ω .
$L^2(\Omega)$	Space of square-integrable functions over Ω ; functions are identified up to equivalence almost everywhere.
$H^m(\Omega)$	Sobolev space of order m , consisting of functions φ such that: $\varphi \in L^2(\Omega)$, $\frac{\partial \varphi}{\partial x_i} \in L^2(\Omega), \dots, D^\alpha \varphi \in L^2(\Omega)$, $\forall \alpha, \alpha \leq m$.
$H_0^m(\Omega)$	$\{\varphi \in H^m(\Omega) \mid D^\alpha \varphi = 0 \text{ on } \Gamma, \forall \alpha \leq m - 1\}$.
$\mathcal{U}$	a Hilbert space on $\mathbb{R}^d$
$\mathcal{U}_{\text{ad}}$	Set of admissible controls; assumed to be a closed and convex subset of the control space $\mathcal{U}$.
$\mathcal{P}(\mathcal{D})$	the set of all open subsets of $\mathcal{D}$ with Lipschitz boundary.

Chapter 2

Optimum Design of Optimal Control Problems for Elasticity

This chapter investigates optimal control problems in both linear elasticity and elastic structures involving contact conditions. The governing state equations are defined in two and three-dimensional spatial domains, and the corresponding control problems are formulated through the minimization of objective functionals involving structural response and control effort. The solutions to these problems are characterized via their associated optimality systems, which consist of two coupled elasticity problems (the state and adjoint equations) together with the necessary optimality condition. The optimal control Abdelbari et al., 2020; Gong and Zhang, 2024 is obtained directly from this system, and the minimized value of the objective functional serves as the basis for subsequent shape and topology optimization, collectively referred to as the optimum design of control systems.

To analyze the sensitivity of the optimal value with respect to geometric variations, both shape gradients and topological derivatives of the control-based objective functional are derived. These differential quantities provide the foundational tools for geometry-driven structural design.

Three numerical methods are proposed to solve the resulting optimum design problems Bourdin and Chambolle, 2003, addressing both smooth and topological geometric changes. Several benchmark examples are presented to demonstrate the effectiveness of the methods, and the corresponding computational results are summarized in this chapter.

2.1 Linear elastic model and boundary control settings

We consider a homogeneous and isotropic elastic body that occupies a bounded domain $\Omega \subset \mathbb{R}^d$, with $d = 2$ or 3 . To facilitate the use of Sobolev space theory, the domain Ω is assumed to have a Lipschitz continuous boundary. Under the small-strain assumption, the geometric deformation of the elastic body is described by a displacement field $\mathbf{u} : \Omega \rightarrow \mathbb{R}^d$, where $\mathbf{u}(x)$ denotes the displacement vector of the material point $x \in \Omega$.

In the framework of linear elasticity, the strain tensor $\boldsymbol{\varepsilon}(\mathbf{u})$ is defined as the symmetric gradient of the displacement:

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2} (\nabla \mathbf{u} + (\nabla \mathbf{u})^\top), \quad (2.1)$$

which characterizes local elongation and shear. The stress tensor $\boldsymbol{\sigma}(\mathbf{u})$ is related to the strain via a linear constitutive law:

$$\boldsymbol{\sigma}(\mathbf{u}) = \mathbb{C} : \boldsymbol{\varepsilon}(\mathbf{u}), \quad (2.2)$$

where $\mathbb{C}$ is the fourth-order stiffness tensor, assumed to be bounded and uniformly positive definite throughout the domain. For isotropic materials, Hooke's law simplifies the relation to:

$$\boldsymbol{\sigma}(\mathbf{u}) = 2\mu \boldsymbol{\varepsilon}(\mathbf{u}) + \lambda \operatorname{tr}(\boldsymbol{\varepsilon}(\mathbf{u})) \mathbf{I}, \quad (2.3)$$

with λ and μ denoting the Lamé parameters, $\operatorname{tr}(\cdot)$ the trace operator, and $\mathbf{I}$ the identity tensor.

To introduce boundary control, the boundary $\partial\Omega$ is partitioned into three mutually disjoint parts:

$$\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma, \quad (2.4)$$

where Γ_D corresponds to a fixed displacement (Dirichlet) boundary, Γ_N denotes the portion where control loads are applied, and Γ is the free boundary where no external forces act. Given the unit outward normal vector $\mathbf{n}$, the boundary conditions are specified as:

$$\begin{cases} \mathbf{u} = 0, & \text{on } \Gamma_D, \\ \boldsymbol{\sigma}(\mathbf{u}) \mathbf{n} = \mathbf{g}, & \text{on } \Gamma_N, \\ \boldsymbol{\sigma}(\mathbf{u}) \mathbf{n} = 0, & \text{on } \Gamma, \end{cases} \quad (2.5)$$

where $\mathbf{g}$ represents the boundary traction applied on Γ_N , regarded as the control variable in the optimization process. The objective is to determine a suitable distribution of $\mathbf{g}$ that drives the structure toward a desired deformation state.

Under static equilibrium, the internal stress field must satisfy the momentum balance equation in strong form:

$$-\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}) = \mathbf{f} \quad \text{in } \Omega, \quad (2.6)$$

where $\mathbf{f}$ denotes the body force density. Together with the prescribed boundary conditions, this system describes the mechanical response of the structure under a given control input and serves as the state equation in the optimal control formulation.

2.2 Function spaces and weak formulation

To rigorously formulate the boundary control problem in the framework of variational analysis, we introduce the necessary function spaces. The admissible displacement fields are taken from the Sobolev space $H^1(\Omega)^d$, which consists of vector-valued functions with square-integrable components and weak derivatives. To account for the homogeneous Dirichlet condition on Γ_D , we define the space of test functions:

$$\mathbf{V}(\Omega) := \{ \mathbf{v} \in H^1(\Omega)^d \mid \mathbf{v} = 0 \text{ on } \Gamma_D \}, \quad (2.7)$$

which is a closed subspace of $H^1(\Omega)^d$ and serves as the solution space for the variational formulation.

We assume the control input $\mathbf{g}$ belongs to the Hilbert space $\mathcal{U} := L^2(\Gamma_N)^d$, and admissible controls lie in a closed, convex subset $\mathcal{U}_{\text{ad}} \subset \mathcal{U}$. This setting allows one to incorporate box constraints or other application-specific control limitations.

Introducing the bilinear form

$$a(\mathbf{u}, \boldsymbol{\psi}) := \int_{\Omega} \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\boldsymbol{\psi}) dx, \quad (2.8)$$

and the linear form (the duality pairing on Γ_N) associated with the control input:

$$\langle \mathbf{g}, \boldsymbol{\psi} \rangle_{\Gamma_N} := \int_{\Gamma_N} \mathbf{g} \cdot \boldsymbol{\psi} ds, \quad (2.9)$$

we obtain the weak form of the linear elasticity system with boundary control:

Find $\mathbf{u} \in \mathbf{V}(\Omega)$ such that

$$a(\mathbf{u}, \boldsymbol{\psi}) = \langle \mathbf{g}, \boldsymbol{\psi} \rangle_{\Gamma_N}, \quad \forall \boldsymbol{\psi} \in \mathbf{V}(\Omega). \quad (2.10)$$

Under standard assumptions on the elasticity tensor $\mathbb{C}$, such as symmetry, boundedness, and uniform ellipticity, the bilinear form $a(\cdot, \cdot)$ is continuous and coercive on $\mathbf{V}(\Omega)$. Therefore, the Lax–Milgram theorem guarantees the existence and uniqueness of a weak solution $\mathbf{u} \in \mathbf{V}(\Omega)$ for every admissible control $\mathbf{g} \in \mathcal{U}_{\text{ad}}$.

2.3 Optimal control formulation and first-order optimality system

In the setting described above, the traction force $\mathbf{g}$ prescribed on the Neumann portion of the boundary Γ_N is treated as the control variable. The objective is to determine a suitable distribution of $\mathbf{g}$ that induces a displacement field $\mathbf{u}$ as close as possible to a prescribed target displacement $\mathbf{u}_d$, while simultaneously minimizing the magnitude of the applied traction to avoid unrealistic or excessive boundary loads.

To achieve this balance, we introduce the following quadratic cost functional:

$$I(\mathbf{g}) := \frac{1}{2} \int_{\Omega} |\mathbf{u} - \mathbf{u}_d|^2 dx + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}|^2 ds, \quad (2.11)$$

where $\mathbf{u}$ is the solution to the linear elasticity state equation (in weak form) under the control $\mathbf{g}$ and $\beta > 0$ is a regularization parameter used to penalize the magnitude of the control. The first term measures the deviation from the desired deformation, and the second term penalizes the control effort.

The optimal control problem can thus be formulated as:

$$\min_{\mathbf{g} \in \mathcal{U}_{\text{ad}}} I(\mathbf{g}), \quad (2.12)$$

where $\mathcal{U}_{\text{ad}} \subset L^2(\Gamma_N)^d$ is a convex and closed admissible set of controls.

2.3.1 Lagrangian approach and derivation of optimality system

To derive the first-order necessary optimality conditions (Karush-Kuhn-Tucker conditions), we adopt the Lagrangian framework. Define a Lagrangian as

$$\mathcal{L}(\mathbf{v}, \mathbf{q}, \mathbf{h}) := \frac{1}{2} \int_{\Omega} |\mathbf{v} - \mathbf{u}_d|^2 dx + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{h}|^2 ds + a(\mathbf{v}, \mathbf{q}) - \langle \mathbf{h}, \mathbf{q} \rangle_{\Gamma_N}, \quad (2.13)$$

where $\mathbf{v}$ is the state variable, $\mathbf{q}$ is the adjoint variable, and $\mathbf{h}$ represents the control. At the optimal solution $(\mathbf{u}, \mathbf{p}, \mathbf{g})$, the partial derivatives of $\mathcal{L}$ with respect to each variable must vanish.

Variation with respect to the adjoint variable $\mathbf{q}$ recovers the state equation:

$$a(\mathbf{u}, \phi) = \langle \mathbf{g}, \phi \rangle_{\Gamma_N}, \quad \forall \phi \in \mathbf{V}(\Omega). \quad (2.14)$$

Variation with respect to the state variable $\mathbf{v}$ yields the adjoint equation:

$$a(\boldsymbol{\psi}, \mathbf{p}) = - \int_{\Omega} (\mathbf{u} - \mathbf{u}_d) \cdot \boldsymbol{\psi} dx, \quad \forall \boldsymbol{\psi} \in \mathbf{V}(\Omega). \quad (2.15)$$

Variation with respect to the control $\mathbf{h}$ leads to the optimality condition:

$$\int_{\Gamma_N} (\beta \mathbf{g} + \mathbf{p}) \cdot \boldsymbol{\phi} ds = 0, \quad \forall \boldsymbol{\phi} \in L^2(\Gamma_N)^d, \quad (2.16)$$

which implies that

$$\mathbf{g} = -\frac{1}{\beta} \mathbf{p} \quad \text{almost everywhere on } \Gamma_N. \quad (2.17)$$

Combining the above results, the first-order optimality system consists of:

State equation (weak form):

$$\mathbf{u} \in \mathbf{V}(\Omega) : \quad a(\mathbf{u}, \boldsymbol{\psi}) = \langle \mathbf{g}, \boldsymbol{\psi} \rangle_{\Gamma_N}, \quad \forall \boldsymbol{\psi} \in \mathbf{V}(\Omega). \quad (2.18)$$

Adjoint equation (weak form):

$$\mathbf{p} \in \mathbf{V}(\Omega) : \quad a(\boldsymbol{\psi}, \mathbf{p}) = - \int_{\Omega} (\mathbf{u} - \mathbf{u}_d) \cdot \boldsymbol{\psi} dx, \quad \forall \boldsymbol{\psi} \in \mathbf{V}(\Omega). \quad (2.19)$$

Optimality condition:

$$\mathbf{g} = -\frac{1}{\beta} \mathbf{p} \quad \text{on } \Gamma_N. \quad (2.20)$$

Given the coercivity and continuity of the bilinear form $a(\cdot, \cdot)$ (guaranteed by the uniform ellipticity of $\mathbb{C}$), and the convexity of the cost functional, the Lax–Milgram theorem ensures that both the state and adjoint equations admit unique solutions. Moreover, the strict convexity of $I(\mathbf{g})$ guarantees a unique optimal control $\mathbf{g}^* \in \mathcal{U}_{\text{ad}}$.

2.4 Shape sensitivity analysis

In the context of boundary optimal control problems, we aim to understand how the objective functional $\mathcal{J}(\Omega)$ responds to perturbations in the shape of the domain Ω . This sensitivity is crucial when the geometry of the domain itself is considered a design variable, as in structural shape optimization, inverse problems, or material design. Such problems are referred to as shape optimization problems.

The sensitivity of the objective functional with respect to variations in the domain shape is captured by the Eulerian derivative (also called the shape derivative). This concept provides a first-order approximation of the change in $\mathcal{J}(\Omega)$ when the domain

is perturbed infinitesimally in a given direction. More precisely, it measures the rate of change of the functional under a smooth deformation of the domain boundary.

Shape derivatives form the analytical foundation for many gradient-based optimization algorithms. Once the Eulerian derivative is computed, it can be used to define a descent direction in the space of admissible shapes, enabling iterative methods that gradually improve the geometry toward an optimal configuration.

In engineering applications, such as structural mechanics, fluid dynamics, or electromagnetic design, the ability to control and optimize the geometry of the domain based on performance metrics (e.g., displacement, energy dissipation, drag, etc.) is of practical importance. In such scenarios, domain perturbations are often constrained by physical or geometric constraints, such as volume preservation, regularity, or fixed subregions (e.g., clamped boundaries that must not move).

To formalize this, consider a control problem defined over a reference domain $\Omega \subset \mathbb{R}^d$. The domain may depend on a parameter or deformation map, leading to a family of perturbed domains Ω_t defined by smooth deformations. For a fixed boundary control (e.g., traction $\mathbf{g}$), the associated state variable $\mathbf{u}_t$ will depend on the domain Ω_t , and so will the objective $\mathcal{J}(\Omega_t)$.

2.4.1 Domain perturbation and admissible shapes

In order to analyze how the objective functional $\mathcal{J}(\Omega)$ changes under perturbations of the domain Nazarov and Sokolowski, 2003, we must first introduce a rigorous mathematical framework for describing domain deformations. We adopt the perturbation of identity method, which is a widely used approach in shape calculus for defining smooth and admissible changes to the domain geometry.

Let $D \subset \mathbb{R}^d$ be a fixed bounded domain, known as the hold-all domain, such that for all admissible shapes considered during optimization, $\Omega \subset D$ is always satisfied. The set of admissible shapes is then defined as:

$$\mathcal{U}_{\text{ad}} := \{\Omega \subset D \mid \Omega \text{ is open, bounded, and has Lipschitz continuous boundary}\}.$$

This regularity condition ensures that the Sobolev spaces $H^1(\Omega)$ and trace theorems can be applied without pathological behavior.

To generate a smooth deformation of the domain, we consider a family of diffeomorphic mappings F_t , $t \in [0, \varepsilon)$, which smoothly deform each point in Ω with respect to a parameter $t \geq 0$. The family is defined as:

$$F_t(x) := x + t\mathcal{V}(x), \quad \text{for } x \in D, \quad (2.21)$$

where $\mathcal{V} : D \rightarrow \mathbb{R}^d$ is a vector field from the admissible deformation space:

$$\Theta_{\text{ad}} := \{ \mathcal{V} \in W^{1,\infty}(D, \mathbb{R}^d) \mid \mathcal{V} = 0 \text{ on } \Gamma_D \}. \quad (2.22)$$

This condition ensures that the Dirichlet portion of the boundary Γ_D remains fixed under the deformation, preserving the prescribed displacement boundary condition $\mathbf{u} = 0$ on Γ_D .

The perturbed domain and its boundary are then given by:

$$\Omega_t := F_t(\Omega) = \{F_t(x) \mid x \in \Omega\}, \quad \partial\Omega_t := F_t(\partial\Omega), \quad (2.23)$$

with the identity $F_0 = \text{Id}$ recovering the original domain: $\Omega_0 = \Omega$. For sufficiently small $t > 0$, the map F_t is invertible and smooth, ensuring that Ω_t is still a Lipschitz domain and thus remains within $\mathcal{U}_{\text{ad}}$.

Correspondingly, we denote by $\mathbf{u}_t$ the state variable (i.e., the displacement field) defined as the solution of the weak form of the linear elasticity problem over the perturbed domain Ω_t , with boundary control applied on the deformed Neumann portion $F_t(\Gamma_N)$. That is, for each $t \in [0, \varepsilon)$, the boundary control $\mathbf{g}$ is applied on $\Gamma_N^t := F_t(\Gamma_N)$, and the Dirichlet condition remains imposed on the fixed set Γ_D .

For any function $\mathbf{u} \in H^1(\Omega)^d$ with associated function $\mathbf{u}_t \in H^1(\Omega_t)^d$ defined in Ω_t , we define the material derivative at $x \in \Omega$ as (cf. Sokolowski and Zolesio, 1992)

$$\dot{\mathbf{u}}(x) = \lim_{t \rightarrow 0^+} \frac{\mathbf{u}_t(F_t(x)) - \mathbf{u}(x)}{t} \quad (2.24)$$

while the shape derivative of $\mathbf{u}$ at $x \in \Omega$ is given by (cf. Sokolowski and Zolesio, 1992)

$$\mathbf{u}'(x) = \dot{\mathbf{u}}(x) - \nabla \mathbf{u}(x) \cdot \mathcal{V}(x) \quad (2.25)$$

Theorem 2.4.1. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain with boundary decomposition $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma$, where Γ_D, Γ_N are disjoint and of class C^k for $k \geq 2$. Assume the target displacement $\mathbf{u}_d \in H^1(\Omega)^d$ and the control $\mathbf{g} \in L^2(\Gamma_N)^d$ satisfy $\mathbf{g} = \mathbf{p}$ on Γ_N almost everywhere. Let the velocity field $\mathcal{V} \in C^1([0, \varepsilon]; \mathcal{D}^k(\Omega; \mathbb{R}^d))$ vanish on $\Gamma_D \cup \Gamma_N$. Then the weak material derivative of the solution $(\mathbf{u}, \mathbf{p})$ to the optimality system exists in the direction $\mathcal{V}$.*

Proof. Let $F_t(x) := x + t\mathcal{V}(x)$ be a family of diffeomorphisms with $F_0 = \text{Id}$, and define the perturbed domains $\Omega_t := F_t(\Omega)$. Let $\mathbf{u}_t, \mathbf{p}_t$ be the state and adjoint solutions on Ω_t satisfying:

$$a_t(\mathbf{u}_t, \phi_t) = \langle \mathbf{g}, \phi_t \rangle_{\Gamma_{N,t}}, \quad \forall \phi_t \in \mathbf{V}(\Omega_t), \quad (2.26)$$

$$a_t(\psi_t, \mathbf{p}_t) = - \int_{\Omega_t} (\mathbf{u}_t - \mathbf{u}_d \circ F_t) \cdot \psi_t \, dx, \quad \forall \psi_t \in \mathbf{V}(\Omega_t). \quad (2.27)$$

Define the pullback to the reference domain:

$$\mathbf{u}^t := \mathbf{u}_t \circ F_t \in \mathbf{V}(\Omega), \quad \mathbf{p}^t := \mathbf{p}_t \circ F_t \in \mathbf{V}(\Omega). \quad (2.28)$$

Change of variables yields the variational problems on Ω :

$$\int_{\Omega} \mathbb{C} : A(t) \boldsymbol{\varepsilon}(\mathbf{u}^t) : \boldsymbol{\varepsilon}(\boldsymbol{\phi}) J(t) dx = \int_{\Gamma_N} N(t) \mathbf{g} \cdot \boldsymbol{\phi} ds, \quad (2.29)$$

$$\int_{\Omega} \mathbb{C} : A(t) \boldsymbol{\varepsilon}(\boldsymbol{\psi}) : \boldsymbol{\varepsilon}(\mathbf{p}^t) J(t) dx = - \int_{\Omega} J(t) (\mathbf{u}^t - \mathbf{u}_d \circ F_t) \cdot \boldsymbol{\psi} dx, \quad (2.30)$$

for all $\boldsymbol{\phi}, \boldsymbol{\psi} \in \mathbf{V}(\Omega)$.

Here:

$$J(t) = |\det DF_t|, \quad A(t) = J(t)(DF_t)^{-T}(DF_t)^{-1}, \quad N(t) = J(t)|(DF_t)^{-T} \mathbf{n}|. \quad (2.31)$$

Since $\mathcal{V} = 0$ on $\Gamma_D \cup \Gamma_N$, it holds that $F_t = \text{Id}$ on $\Gamma_D \cup \Gamma_N$, so $N(t)|_{\Gamma_N} = 1$, and the right-hand sides are fixed in t .

By uniform ellipticity and continuity of $A(t), J(t)$ and the regularity of the data, the bilinear form remains coercive for t small. Then by the Lax–Milgram theorem, $\mathbf{u}^t, \mathbf{p}^t$ exist uniquely in $H^1(\Omega)^d$ and satisfy:

$$\begin{aligned} \|\mathbf{u}^t\|_{H^1(\Omega)} &\leq C, \\ \|\mathbf{p}^t\|_{H^1(\Omega)} &\leq C \|\mathbf{u}^t - \mathbf{u}_d \circ F_t\|_{L^2(\Omega)} \leq C' (\|\mathbf{u}^t\|_{H^1(\Omega)} + \|\mathbf{u}_d\|_{H^1(\Omega)}) \leq C''. \end{aligned}$$

Define difference quotients:

$$\mathbf{y}_u^t := \frac{\mathbf{u}^t - \mathbf{u}}{t}, \quad \mathbf{y}_p^t := \frac{\mathbf{p}^t - \mathbf{p}}{t}. \quad (2.32)$$

Then we have

$$\begin{aligned} &\int_{\Omega} \mathbb{C} : \boldsymbol{\varepsilon}(\mathbf{y}_u^t) : \boldsymbol{\varepsilon}(\boldsymbol{\phi}) dx + \frac{1}{\beta} \int_{\Gamma_N} \mathbf{y}_p^t \cdot \boldsymbol{\phi} ds \\ &= \frac{1}{t} \left[\int_{\Omega} (\mathbb{C} : (A(t) \boldsymbol{\varepsilon}(\mathbf{u}^t) - \boldsymbol{\varepsilon}(\mathbf{u})) J(t) - \mathbb{C} : \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\boldsymbol{\phi}) dx - \int_{\Gamma_N} (N(t) \mathbf{g} - \mathbf{g}) \cdot \boldsymbol{\phi} ds \right] \end{aligned} \quad (2.33)$$

and

$$\begin{aligned} &\int_{\Omega} \mathbb{C} : \boldsymbol{\varepsilon}(\boldsymbol{\psi}) : \boldsymbol{\varepsilon}(\mathbf{y}_p^t) dx = \\ &\quad - \frac{1}{t} \int_{\Omega} [(J(t) - 1) (\mathbf{u}^t - \mathbf{u}_d \circ F_t) + J(t) (\mathbf{u}_d \circ F_t - \mathbf{u}_d)] \cdot \boldsymbol{\psi} dx - \int_{\Omega} (\mathbf{y}_u^t \cdot \boldsymbol{\psi}) dx \end{aligned} \quad (2.34)$$

Subtracting the variational forms at $t > 0$ and $t = 0$, dividing by t , and using the known expansions (cf. Sokolowski and Zolesio, 1992):

$$\frac{A(t) - I}{t} \rightarrow (\nabla \cdot \mathcal{V})I - \nabla \mathcal{V} - \nabla \mathcal{V}^T, \quad \frac{J(t) - 1}{t} \rightarrow \nabla \cdot \mathcal{V}, \quad (2.35)$$

we deduce that $\mathbf{y}_u^t, \mathbf{y}_p^t$ are bounded in $H^1(\Omega)^d$ and hence converge weakly to limits:

$$\mathbf{y}_u^t \rightharpoonup \dot{\mathbf{u}}, \quad \mathbf{y}_p^t \rightharpoonup \dot{\mathbf{p}} \quad \text{in } H^1(\Omega)^d \quad \text{as } t \rightarrow 0^+. \quad (2.36)$$

Thus, the material derivatives $\dot{\mathbf{u}}, \dot{\mathbf{p}}$ exist in the weak sense. This completes the proof. $\square$

Lemma 2.4.2. *For a function $\phi(t, x) \in C([0, \tau]; W_{loc}^{1,1}(\mathbb{R}^d)^d) \cap C^1([0, \tau]; L_{loc}^1(\mathbb{R}^d)^d)$, the Eulerian derivative of the integral functional*

$$F(\Omega) = \int_{\Omega} \mathbf{f}_1(x) dx \quad (2.37)$$

is given by (cf. Delfour and Zolésio, 2011b):

$$dF(\Omega; \mathcal{V}) = \int_{\Omega} (\phi'(0, x) + \operatorname{div}(\phi(0, x)\mathcal{V})) dx. \quad (2.38)$$

Applying Lemma 2.4.2 to the variational formulations of the state and adjoint equations on the perturbed domains Ω_t , differentiating with respect to t at $t = 0$, and then applying Green's formula, we obtain the following reformulated system:

$$\begin{aligned} & \int_{\Omega} \mathbb{C}\boldsymbol{\varepsilon}(\mathbf{u}') : \boldsymbol{\varepsilon}(\mathbf{v}) dx + \int_{\Omega} \operatorname{div}(\mathbb{C}\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) \mathcal{V}) dx \\ &= -\frac{1}{\beta} \int_{\Gamma_N} \mathbf{p}' \cdot \mathbf{v} ds + \frac{1}{\beta} \int_{\Gamma_N} (\mathcal{V} \cdot \mathbf{n}) \mathbf{p} \cdot \mathbf{v} ds, \end{aligned} \quad (2.39)$$

and

$$\begin{aligned} & \int_{\Omega} \mathbb{C}\boldsymbol{\varepsilon}(\mathbf{p}') : \boldsymbol{\varepsilon}(\mathbf{w}) dx + \int_{\Omega} \operatorname{div}(\mathbb{C}\boldsymbol{\varepsilon}(\mathbf{p}) : \boldsymbol{\varepsilon}(\mathbf{w}) \mathcal{V}) dx \\ &= - \int_{\Omega} \mathbf{u}' \cdot \mathbf{w} dx - \int_{\Omega} \operatorname{div}((\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{w} \mathcal{V}) dx. \end{aligned} \quad (2.40)$$

Using the divergence theorem and assuming $\mathcal{V}|_{\Gamma_D \cup \Gamma_N} = 0$, the system reduces to

a coupled boundary value problem for the shape derivatives $(\mathbf{u}', \mathbf{p}')$:

$$\left\{ \begin{array}{ll} -\operatorname{div}(\mathbb{C}\varepsilon(\mathbf{u}')) = \mathbf{0} & \text{in } \Omega, \\ -\operatorname{div}(\mathbb{C}\varepsilon(\mathbf{p}')) = \mathbf{u}' & \text{in } \Omega, \\ \mathbf{u}' = \mathbf{0} & \text{on } \Gamma_D, \\ \mathbf{p}' = \mathbf{0} & \text{on } \Gamma_D, \\ \mathbb{C}\varepsilon(\mathbf{u}') \cdot \mathbf{n} = -\frac{1}{\beta}\mathbf{p}' & \text{on } \Gamma_N, \\ \mathbb{C}\varepsilon(\mathbf{p}') \cdot \mathbf{n} = \mathbf{u}' & \text{on } \Gamma_N. \end{array} \right. \quad (2.41)$$

For all $t \in [0, \tau]$ and $\phi_1, \phi_2, \psi \in H^1(\Omega_t)^d$, we define the Lagrangian functional associated with the linear elasticity optimal control problem as follows:

$$\begin{aligned} \mathcal{L}(\Omega_t, \phi_1, \phi_2, \psi) = & \frac{1}{2} \int_{\Omega_t} |\phi_1 - \mathbf{u}_d|^2 dx + \frac{\beta}{2} \int_{\Gamma_{N,t}} |\phi_2|^2 ds \\ & + \int_{\Omega_t} \mathbb{C}\varepsilon(\phi_1) : \varepsilon(\psi) dx - \int_{\Gamma_{N,t}} \phi_2 \cdot \psi ds \end{aligned} \quad (2.42)$$

Calculating the first-order optimality conditions of this Lagrangian, we obtain:

$$\begin{aligned} \frac{\partial \mathcal{L}(\Omega_t, \mathbf{u}_t, \mathbf{g}_t, \mathbf{p}_t)}{\partial \mathbf{u}_t} [\delta \mathbf{u}] &= 0, \quad \frac{\partial \mathcal{L}(\Omega_t, \mathbf{u}_t, \mathbf{g}_t, \mathbf{p}_t)}{\partial \mathbf{g}_t} [\delta \mathbf{g}] = 0, \\ \frac{\partial \mathcal{L}(\Omega_t, \mathbf{u}_t, \mathbf{g}_t, \mathbf{p}_t)}{\partial \mathbf{p}_t} [\delta \mathbf{p}] &= 0. \end{aligned} \quad (2.43)$$

for any $\delta \mathbf{u}, \delta \mathbf{p}, \delta \mathbf{g} \in H^1(\Omega_t)$

From the first-order optimality conditions of the Lagrangian functional, we know that the solution $(\mathbf{u}_t, \mathbf{g}_t, \mathbf{p}_t)$ satisfies the saddle point condition. Hence, the objective functional $J(\Omega_t)$ admits the representation:

$$J(\Omega_t) = \min_{(\phi_1, \phi_2)} \max_{\psi} \mathcal{L}(\Omega_t, \phi_1, \phi_2, \psi), \quad (2.44)$$

where:

- ϕ_1 represents the state variable candidate,
- ϕ_2 is the control candidate,
- ψ is the adjoint test variable,
- and all functions lie in $H^1(\Omega_t)^d$.

To compute the shape derivative of $J(\Omega_t)$, we use a change-of-variable (pullback) transformation. Specifically, we introduce the parametrized (pullback) space on the fixed reference domain Ω :

$$H^1(\Omega_t)^d = \{ \phi \circ F_t^{-1} : \phi \in H^1(\Omega)^d \}. \quad (2.45)$$

Accordingly, we define the pullback Lagrangian on the fixed domain Ω as:

$$\hat{\mathcal{L}}(t, \phi_1, \phi_2, \psi) := \mathcal{L}(F_t(\Omega)[\mathcal{V}], \phi_1 \circ F_t^{-1}, \phi_2 \circ F_t^{-1}, \psi \circ F_t^{-1}), \quad (2.46)$$

with $\phi_1, \phi_2, \psi \in H^1(\Omega)^d$.

Let $(\mathbf{u}, \mathbf{g}, \mathbf{p})$ denote the solution to the optimality system on the reference domain Ω (i.e., at $t = 0$). Then, by Céa's method(cf. Céa, 1971), the Eulerian derivative of the cost functional can be computed as the derivative of the pullback Lagrangian at this saddle point:

$$dJ(\Omega; \mathcal{V}) = \min_{(\phi_1, \phi_2)} \max_{\psi} \frac{d}{dt} \hat{\mathcal{L}}(t, \phi_1, \phi_2, \psi) \Big|_{t=0} = \frac{d}{dt} \hat{\mathcal{L}}(t, \mathbf{u}, \mathbf{g}, \mathbf{p}) \Big|_{t=0}, \quad (2.47)$$

for all admissible velocity fields $\mathcal{V} \in \mathcal{U} := \{ \mathcal{V} \in \mathbf{W}^{1,\infty}(\Omega)^d : \mathcal{V}|_{\Gamma_D \cup \Gamma_N} = \mathbf{0} \}$.

This result is rigorously justified due to the shape differentiability of the state equation, which has been established in Theorem 2.4.1.

Next, we compute the Eulerian derivative of the shape functional for the linear elasticity control problem. Assuming that the deformation field satisfies $\mathcal{V}|_{\Gamma_D \cup \Gamma_N} = 0$, we express the Lagrangian $\hat{\mathcal{L}}$, originally defined on the perturbed domain Ω_t , on the fixed domain Ω :

$$\begin{aligned} \hat{\mathcal{L}}(t, \phi_1, \phi_2, \psi) &= \frac{1}{2} \int_{\Omega} J(t) |\phi_1 - \mathbf{u}_d|^2 dx + \frac{\beta}{2} \int_{\Gamma_N} N(t) |\phi_2|^2 ds \\ &\quad + \int_{\Omega} A(t) (\mathbb{C}\varepsilon(\phi_1) : \varepsilon(\psi)) dx - \int_{\Gamma_N} N(t) \phi_2 \cdot \psi ds. \end{aligned} \quad (2.48)$$

Taking the partial derivative of the pulled-back Lagrangian $\hat{\mathcal{L}}$ with respect to t , and applying shape calculus identities (e.g., differentiating through the Jacobian $J(t)$,

we obtain the Eulerian derivative:

$$\begin{aligned}
\partial_t \hat{\mathcal{L}}(t, \phi_1, \phi_2, \psi) \Big|_{t=0} &= \int_{\Omega} \operatorname{div}(\mathcal{V}) \cdot \frac{1}{2} |\phi_1 - \mathbf{u}_d|^2 dx \\
&+ \int_{\Omega} [\operatorname{div}(\mathcal{V}) \mathbb{C} \boldsymbol{\varepsilon}(\phi_1) - \mathbb{C} (\nabla \mathcal{V}^T \boldsymbol{\varepsilon}(\phi_1) + \boldsymbol{\varepsilon}(\phi_1) \nabla \mathcal{V})] : \boldsymbol{\varepsilon}(\psi) dx \\
&+ \beta \int_{\Gamma_N} (\operatorname{div} \mathcal{V} - D\mathcal{V} \mathbf{n} \cdot \mathbf{n}) \cdot \frac{1}{2} |\phi_2|^2 ds \\
&- \int_{\Gamma_N} (\operatorname{div} \mathcal{V} - D\mathcal{V} \mathbf{n} \cdot \mathbf{n}) \cdot \phi_2 \cdot \psi ds
\end{aligned} \tag{2.49}$$

Then, evaluating this derivative at the saddle point $(\mathbf{u}, \mathbf{g}, \mathbf{p})$, we get the shape derivative:

$$\begin{aligned}
dJ(\Omega; \mathcal{V}) &= \int_{\Omega} \left[\frac{1}{2} |\mathbf{u} - \mathbf{u}_d|^2 \operatorname{div} \mathcal{V} + (\operatorname{div} \mathcal{V} \cdot \boldsymbol{\sigma}(\mathbf{u}) - \boldsymbol{\sigma}(\mathbf{u}) \cdot \nabla \mathcal{V} - \nabla \mathcal{V}^T \cdot \boldsymbol{\sigma}(\mathbf{u})) : \boldsymbol{\varepsilon}(\mathbf{p}) \right] \\
&+ \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}|^2 (\operatorname{div} \mathcal{V} - D\mathcal{V} \mathbf{n} \cdot \mathbf{n}) ds - \int_{\Gamma_N} (\operatorname{div} \mathcal{V} - D\mathcal{V} \mathbf{n} \cdot \mathbf{n}) \cdot \mathbf{g} \cdot \mathbf{p} ds
\end{aligned} \tag{2.50}$$

We now convert the volume integrals into boundary integrals by applying Green's formula and standard identities from shape calculus. In particular, we use the following identity:

$$\int_{\Omega} (\operatorname{div} \mathcal{V}) f dx = \int_{\partial\Omega} f (\mathcal{V} \cdot \mathbf{n}) ds - \int_{\Omega} \nabla f \cdot \mathcal{V} dx, \tag{2.51}$$

as well as the shape derivative identity for the bilinear term involving $\boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{p})$ and $\mathcal{V}|_{\Gamma_D \cup \Gamma_N} = 0$, which yields:

$$dJ(\Omega; \mathcal{V}) = \int_{\Gamma} \left(\frac{1}{2} |\mathbf{u} - \mathbf{u}_d|^2 + \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{p}) \right) (\mathcal{V} \cdot \mathbf{n}) ds \tag{2.52}$$

After deriving the shape derivative and its boundary (surface) expression, we now proceed to the topological sensitivity analysis. Unlike the shape derivative, which measures the effect of infinitesimal deformations of the domain boundary, the topological derivative Sokolowski and Zochowski, 1999a; Sokolowski and Zochowski, 1999b quantifies the variation of the objective functional due to the insertion of a small hole (or inclusion) inside the domain Ω . Therefore, it captures the sensitivity of the functional with respect to local topological changes within the domain, such as material removal or inclusion, which is particularly relevant in structural optimization problems involving material layout, void nucleation, or crack initiation. In the following, we formulate the corresponding perturbation model and derive an analytical expression for the topological derivative.

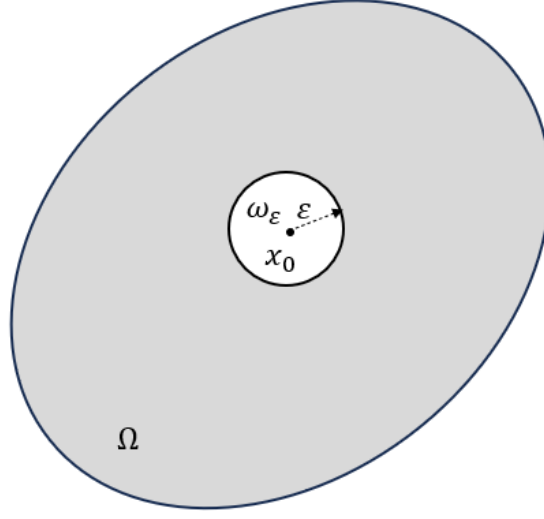


Figure 2.1: Example of topological perturbation

2.5 Topological sensitivity

Domain decomposition techniques together with the Steklov-Poincaré pseudo-differential boundary operator are usually used for topological asymptotic analysis in the nucleation of small circular inclusions Novotny et al., 2019d; Novotny and Sokolowski, 2013, 2020. Let us consider an open and bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 2, 3$), which is subject to a nonsmooth perturbation confined in a small region $\omega_\varepsilon(x_0) = x_0 + \varepsilon\omega$ of size ε , with $\overline{\omega_\varepsilon} \Subset \Omega$, as shown in Fig. 2.1. Here, x_0 is an arbitrary point of Ω and ω is a fixed domain of $\mathbb{R}^d$.

Define the singular perturbation of Ω , denote $\Omega_\varepsilon := \Omega \setminus \overline{\omega_\varepsilon}$. Now, let us state the same optimality system in the perturbed domain Ω_ε : $\forall \psi \in \mathbf{V}(\Omega_\varepsilon)$

$$\mathbf{u}_\varepsilon \in \mathbf{V}(\Omega_\varepsilon) : \quad \int_{\Omega} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon) : \boldsymbol{\varepsilon}(\psi) = \int_{\Gamma_N} \mathbf{g}_\varepsilon \cdot \psi, \quad (2.53)$$

$$\mathbf{p}_\varepsilon \in \mathbf{V}(\Omega_\varepsilon) : \quad \int_{\Omega} \boldsymbol{\sigma}(\mathbf{p}_\varepsilon) : \boldsymbol{\varepsilon}(\psi) = - \int_{\Omega_\varepsilon} (\mathbf{u}_\varepsilon - \mathbf{u}_d) \cdot \psi, \quad (2.54)$$

$$\mathbf{g}_\varepsilon = -\frac{1}{\beta} \mathbf{p}_\varepsilon \text{ on } \Gamma_N. \quad (2.55)$$

The shape functional in Ω_ε

$$\mathcal{J}_\varepsilon(\Omega) = \inf_{\mathbf{h} \in L^2(\Gamma_N)^d} I_\varepsilon(\mathbf{h}) = I_\varepsilon(\mathbf{g}_\varepsilon) \quad (2.56)$$

then we can know

$$\mathcal{J}_\varepsilon(\Omega) = \frac{1}{2} \int_{\Omega_\varepsilon} |\mathbf{u}_\varepsilon - \mathbf{u}_d|^2 + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}_\varepsilon|^2. \quad (2.57)$$

Now we consider decomposing Ω_ε into two parts, namely $\Omega_\varepsilon = \Omega_R \cup \overline{C(R, \varepsilon)}$, where $\Omega_R := \Omega_\varepsilon \setminus \overline{C(R, \varepsilon)}$ and $C(R, \varepsilon)$ with the outer boundary ∂B_R denotes a ball of radius $R > 0$ centered at an arbitrary point $x_0 \in \Omega$ and there is a hole ω_ε inside of $C(R, \varepsilon)$ and $R \gg \varepsilon > 0$.

We determine the family of Steklov-Poincaré boundary operators on the outer boundary ∂B_R of the domain $C(R, \varepsilon)$. For the boundary value problem defined in Ω_ε , we introduce the truncated problem in Ω_R . The singular perturbation Ω_ε of the geometrical domain Ω is replaced by a regular perturbation of the Steklov-Poincaré boundary operator living on the interface, which coincides with the interior boundary ∂B_R of Ω_R .

Definition 2.5.1. *The Steklov-Poincaré boundary operator*

$$\mathcal{S}_\varepsilon : H^{1/2}(\partial B_R) \rightarrow H^{-1/2}(\partial B_R) \quad (2.58)$$

is defined for the elasticity equation in the domain $C(R, \varepsilon)$. For a fixed parameter $\varepsilon > 0$ and a given element $\mathbf{v} \in H^{1/2}(\partial B_R)$ the corresponding element in the range of the operator $\mathcal{S}_\varepsilon$ is given by the Neumann trace of a unique solution to the boundary value problem

$$\text{Find } \mathbf{w}_\varepsilon \text{ such that } \begin{cases} -\operatorname{div}(\boldsymbol{\sigma}(\mathbf{w}_\varepsilon)) = 0 & \text{in } C(R, \varepsilon) \\ \mathbf{w}_\varepsilon = \mathbf{v} & \text{on } \partial B_R \\ \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) \cdot \mathbf{n} = 0 & \text{on } \partial \omega_\varepsilon. \end{cases} \quad (2.59)$$

Then we set

$$\mathcal{S}_\varepsilon(\mathbf{v}) = \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) \cdot \boldsymbol{\nu} \quad \text{on } \partial B_R, \quad (2.60)$$

here $\boldsymbol{\nu}$ is the unit exterior normal vector on $\partial C(R, \varepsilon)$ and $\boldsymbol{\nu} = -\mathbf{n}$. If $\mathbf{v} = \mathbf{u}_\varepsilon|_{\partial B_R}$ we have $\mathbf{w}_\varepsilon = \mathbf{u}_\varepsilon|_{C(R, \varepsilon)}$ and $\mathbf{u}_\varepsilon^R = \mathbf{u}_\varepsilon|_{\Omega_R}$, where $\mathbf{u}_\varepsilon$ is the solution of the perturbed problem in Ω_ε .

Notice that by the definition of operator $\mathcal{S}_\varepsilon$, the solution $\mathbf{w}_\varepsilon$ of (2.59) satisfies:

$$\int_{C(R, \varepsilon)} \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) : \boldsymbol{\varepsilon}(\mathbf{w}_\varepsilon) = \int_{\partial B_R} \mathcal{S}_\varepsilon(\boldsymbol{\psi}) \cdot \boldsymbol{\psi}. \quad (2.61)$$

By the Novotny and Sokolowski, 2020, we know the Steklov-Poincaré operator for the ring $C(R, \varepsilon)$ admits the expansion for $\varepsilon > 0, \varepsilon$ small enough,

$$\mathcal{S}_\varepsilon = \mathcal{S} + \varepsilon^d \mathcal{S}_1 + \mathcal{R}_\varepsilon, \quad (2.62)$$

where the remainder $\mathcal{R}_\varepsilon$ is of order $o(\varepsilon^d)$ in the operator norm $\mathcal{L}(H^{1/2}(\partial B_R); H^{-1/2}(\partial B_R))$.

Theorem 2.5.2. *The topological derivative of the cost functional (2.57) is*

$$\mathcal{T}(\hat{x}) = -\mathbb{P}_r \boldsymbol{\sigma}(\mathbf{u}(\hat{x})) : \boldsymbol{\varepsilon}(\mathbf{p}(\hat{x})). \quad (2.63)$$

Proof. We consider the state equation in Ω_R by $\mathcal{S}_\varepsilon$: Find $\mathbf{u}_\varepsilon^R \in \mathbf{V}(\Omega_R)$, such that for $\forall \mathbf{v} \in \mathbf{V}(\Omega_R)$,

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon^R) : \mathbf{e}(\mathbf{v}) + \langle \mathcal{S}_\varepsilon(\mathbf{u}_\varepsilon^R), \mathbf{v} \rangle_{\partial B_R} = \langle \mathbf{g}_\varepsilon^R, \mathbf{v} \rangle_{\Gamma_N}, \quad (2.64)$$

and we denote

$$a(\Omega_R; \mathbf{u}_\varepsilon^R, \mathbf{v}) := \int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon^R) : \mathbf{e}(\mathbf{v}) \quad (2.65)$$

Also, the adjoint equation in Ω_R by $\mathcal{S}_\varepsilon$: Find $\mathbf{p}_\varepsilon^R \in \mathbf{V}(\Omega_R)$, such that for $\forall \mathbf{v} \in \mathbf{V}(\Omega_R)$,

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{p}_\varepsilon^R) : \mathbf{e}(\mathbf{v}) + \langle \mathcal{S}_\varepsilon(\mathbf{p}_\varepsilon^R), \mathbf{v} \rangle_{\partial B_R} = - \int_{\Omega} (\mathbf{u}_\varepsilon^R - \mathbf{u}_d) \mathbf{v}. \quad (2.66)$$

This Steklov-Poincaré operator can be also used for Ω_R , then we have

$$\mathcal{S}_\varepsilon(\mathbf{u}_\varepsilon^R) = \sigma(\mathbf{u}_\varepsilon^R) \mathbf{n} = \mathcal{S}_\varepsilon(\mathbf{v}) = \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) \boldsymbol{\nu} \quad \text{on } \partial B_R, \quad (2.67)$$

where $\mathbf{w}_\varepsilon|_{\partial B_R} = \mathbf{u}_\varepsilon^R|_{\partial B_R}$. In (2.61), by Green's formula of integration by parts, we can get

$$a(C(R, \varepsilon); \mathbf{w}_\varepsilon, \mathbf{w}_\varepsilon) = \langle \mathcal{S}_\varepsilon(\mathbf{w}_\varepsilon), \mathbf{w}_\varepsilon \rangle_{\partial B_R} = - \langle \mathcal{S}_\varepsilon(\mathbf{u}_\varepsilon^R), \mathbf{u}_\varepsilon^R \rangle_{\partial B_R}, \quad (2.68)$$

where $\mathbf{u}_\varepsilon^R$ in Ω_R and $\mathbf{w}_\varepsilon$ in $C(R, \varepsilon)$.

It is well known that the topological asymptotic expansion for the energy functional takes the following form Novotny and Sokolowski, 2013:

$$\int_{C(R, \varepsilon)} \boldsymbol{\sigma}(\mathbf{v}_\varepsilon) : \boldsymbol{\varepsilon}(\mathbf{v}_\varepsilon) = \int_{B_R} \boldsymbol{\sigma}(\mathbf{v}) : \boldsymbol{\varepsilon}(\mathbf{v}) + \varepsilon^d \mathbb{P}_r \boldsymbol{\sigma}(\mathbf{v}) : \boldsymbol{\varepsilon}(\mathbf{v}) + o(\varepsilon^d), \quad (2.69)$$

where $\mathbf{v} = \mathbf{u}|_{B_R}$ is the solution to the unperturbed problem and $\mathbb{P}_r$ is the Pólya-Szegő polarization tensor Ammari and Kang, 2007. According to the expansion given in (2.62) and by the symmetry of the Steklov-Poincaré operator, the expansion of the energy functional can also be written as

$$\langle \mathcal{S}_\varepsilon(\boldsymbol{\varphi}), \boldsymbol{\vartheta} \rangle = \langle \mathcal{S}(\boldsymbol{\varphi}), \boldsymbol{\vartheta} \rangle + \varepsilon^d \langle \mathcal{S}_1(\boldsymbol{\varphi}), \boldsymbol{\vartheta} \rangle + \langle \mathcal{R}_\varepsilon(\boldsymbol{\varphi}), \boldsymbol{\vartheta} \rangle, \quad (2.70)$$

where $\langle \mathcal{R}_\varepsilon(\boldsymbol{\varphi}), \boldsymbol{\vartheta} \rangle = o(\varepsilon^d)$. Then, we have topological derivative of the energy in $C(R, \varepsilon) \subset \mathbb{R}^d$.

$$a(C(R, \varepsilon); \boldsymbol{\psi}_\varepsilon, \boldsymbol{\psi}_\varepsilon) = a(B_R; \boldsymbol{\psi}, \boldsymbol{\psi}) + \varepsilon^d \langle \mathbb{P}_r \boldsymbol{\sigma}(\boldsymbol{\psi}), \boldsymbol{\varepsilon}(\boldsymbol{\psi}) \rangle + o(\varepsilon^d). \quad (2.71)$$

From (2.68), we get

$$-\langle \mathcal{S}_\varepsilon(\mathbf{u}_\varepsilon^R), \mathbf{u}_\varepsilon^R \rangle_{\partial B_R} = a(B_R; \mathbf{u}|_{B_R}, \mathbf{u}|_{B_R}) + \varepsilon^d \langle \mathbb{P}_r \boldsymbol{\sigma}(\mathbf{u}), \boldsymbol{\varepsilon}(\mathbf{u}) \rangle + o(\varepsilon^d). \quad (2.72)$$

Then, we get

$$\langle \mathcal{S}_1(\boldsymbol{\varphi}), \boldsymbol{\vartheta} \rangle = -\mathbb{P}_r \boldsymbol{\sigma}(\boldsymbol{\varphi}(\hat{x})) : \boldsymbol{\varepsilon}(\boldsymbol{\vartheta}(\hat{x})) \quad \forall \hat{x} \in \Omega. \quad (2.73)$$

We consider the following ansätze for the solutions $\mathbf{u}_\varepsilon, \mathbf{p}_\varepsilon, \mathbf{g}_\varepsilon$ to the topologically perturbed coupled system (2.53), (2.54), (2.55):

$$\begin{aligned} \mathbf{u}_\varepsilon &= \mathbf{u} + \varepsilon^d \mathbf{u}_1 + \tilde{\mathbf{u}}_\varepsilon, \\ \mathbf{p}_\varepsilon &= \mathbf{p} + \varepsilon^d \mathbf{p}_1 + \tilde{\mathbf{p}}_\varepsilon, \\ \mathbf{g}_\varepsilon &= \mathbf{g} + \varepsilon^d \mathbf{g}_1 + \tilde{\mathbf{g}}_\varepsilon, \end{aligned} \quad (2.74)$$

where $\mathbf{u}, \mathbf{p}, \mathbf{g}$ are solutions to the unperturbed coupled system (2.18), (2.19), (2.20); $\mathbf{u}_1, \mathbf{p}_1, \mathbf{g}_1$ are the first-order asymptotic correction terms and $\tilde{\mathbf{u}}_\varepsilon, \tilde{\mathbf{p}}_\varepsilon, \tilde{\mathbf{g}}_\varepsilon$ are the remainders of order $o(\varepsilon^d)$.

We differentiate (2.64) with $\rho = \varepsilon^d$ at $\varepsilon = 0^+$,

$$\mathbf{u} \in V(\Omega_R) : \quad a(\Omega_R; \mathbf{u}_1, \mathbf{v}) + \langle \mathcal{S}(\mathbf{u}_1), \mathbf{v} \rangle_{\partial B_R} + \langle \mathcal{S}_1(\mathbf{u}), \mathbf{v} \rangle_{\partial B_R} = \langle \mathbf{g}_1, \mathbf{v} \rangle_{\Gamma_N}. \quad (2.75)$$

Similarly, we can get

$$\mathbf{u} \in V(\Omega_R) : \quad a(\Omega_R; \mathbf{p}_1, \mathbf{v}) + \langle \mathcal{S}(\mathbf{p}_1), \mathbf{v} \rangle_{\partial B_R} + \langle \mathcal{S}_1(\mathbf{p}), \mathbf{v} \rangle_{\partial B_R} = -\langle \mathbf{u}_1, \mathbf{v} \rangle_{\Gamma_N}. \quad (2.76)$$

and

$$\mathbf{g}_1 = -\frac{1}{\beta} \mathbf{p}_1 \text{ on } \Gamma_N. \quad (2.77)$$

We assume that a given shape functional $\mathcal{J}_\varepsilon(\hat{x})$, associated with the topologically perturbed domain, admits a topological asymptotic expansion of the form

$$\mathcal{J}_\varepsilon(\hat{x}) = \mathcal{J}(\hat{x}) + f(\varepsilon) \mathcal{T}(\hat{x}) + R(f(\varepsilon)), \quad (2.78)$$

where $\mathcal{J}(\hat{x})$ is the shape functional associated with the reference domain, $f(\varepsilon)$ is a positive first-order correction function, which decreases monotonically such that $f(\varepsilon) \rightarrow 0$ with $\varepsilon \rightarrow 0$, and $R(f(\varepsilon))$ is the remainder term, that is, $R(f(\varepsilon))/f(\varepsilon) \rightarrow 0$ with $\varepsilon \rightarrow 0$. The function $\hat{x} \rightarrow \mathcal{T}(\hat{x})$ is recognized as the *topological derivative* of J at $\hat{x}$.

We have the shape functional

$$\mathcal{J}_\varepsilon(\hat{x}) = \frac{1}{2} \int_{\Omega_R} |\mathbf{u}_\varepsilon^R - \mathbf{u}_d|^2 + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}_\varepsilon^R|^2. \quad (2.79)$$

Then we differentiate (2.79) with $\rho = \varepsilon^d$ at $\varepsilon = 0^+$.

$$\mathcal{T}(\hat{x}) = \int_{\Omega_R} (\mathbf{u}^R - \mathbf{u}_d) \cdot \mathbf{u}_1 + \beta \int_{\Gamma_N} \mathbf{g}^R \cdot \mathbf{g}_1. \quad (2.80)$$

Now, let us rewrite the adjoint system as

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{p}) : \boldsymbol{\varepsilon}(\mathbf{v}) + \int_{\partial B_R} \mathcal{S}(\mathbf{p}) \cdot \mathbf{v} = - \int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{v}. \quad (2.81)$$

By taking $\mathbf{u}_1$ as the test functions in (2.81), we have the following equalities:

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{p}) : \boldsymbol{\varepsilon}(\mathbf{u}_1) + \int_{\partial B_R} \mathcal{S}(\mathbf{p}) \cdot \mathbf{u}_1 = - \int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{u}_1. \quad (2.82)$$

On the other hand, by taking $\mathbf{p}$ as the test functions in (2.75), we obtain

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_1) : \boldsymbol{\varepsilon}(\mathbf{p}) + \int_{\partial B_R} (\mathcal{S}_1(\mathbf{u}) + \mathcal{S}(\mathbf{u}_1)) \cdot \mathbf{p} = \int_{\Gamma_N} \mathbf{g}_1 \cdot \mathbf{p} = -\beta \int_{\Gamma_N} \mathbf{g}_1 \cdot \mathbf{g}. \quad (2.83)$$

Combining the above equalities yields the following important result:

$$\int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{u}_1 + \beta \int_{\Gamma_N} \mathbf{g}_1 \cdot \mathbf{g} = \int_{\partial B_R} \mathcal{S}(\mathbf{u}_1) \cdot \mathbf{p} = -\mathbb{P}_r \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{p}). \quad (2.84)$$

Then the topological derivative

$$\mathcal{T}(\hat{x}) = \int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{u}_1 + \beta \int_{\Gamma_N} \mathbf{g} \cdot \mathbf{g}_1 = -\mathbb{P}_r \boldsymbol{\sigma}(\mathbf{u}(\hat{x})) : \boldsymbol{\varepsilon}(\mathbf{p}(\hat{x})). \quad (2.85)$$

□

Building upon the previous analysis of shape and topological sensitivities in the linear elasticity control problem, we now turn our attention to a more physically realistic and technically challenging scenario—where the boundary of the domain is subject to frictional contact conditions. In many engineering applications, such as contact between mechanical components, the assumption of perfect displacement or traction boundaries becomes insufficient. Instead, one must account for unilateral constraints and frictional interactions at the contact interface. To this end, we reformulate the original problem by incorporating contact conditions with friction, and investigate the corresponding variational structure and sensitivity properties under these boundary constraints.

2.6 Optimal control of linear elasticity with frictional boundary contact

In this section, we extend the previous analysis by introducing frictional contact conditions along a portion of the boundary. Specifically, we consider a linear elasticity problem in a bounded domain $\Omega \subset \mathbb{R}^2$, where the boundary $\partial\Omega$ is decomposed as $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_C$, with Γ_D , Γ_N , and Γ_C representing the Dirichlet, Neumann, and frictional contact boundaries, respectively. The goal is to minimize the control cost while accounting for the unilateral contact and frictional interaction along Γ_C .

Let $\mathbf{u} \in H^1(\Omega; \mathbb{R}^2)$ denote the displacement field governed by the following contact problem (see, e.g., Chaudet-Dumas, 2023; Chaudet-Dumas and Deteix, 2021):

$$\begin{aligned} -\operatorname{div}(\boldsymbol{\sigma}) &= 0 && \text{in } \Omega, \\ \mathbf{u} &= 0 && \text{on } \Gamma_D, \\ \boldsymbol{\sigma} \cdot \mathbf{n} &= \mathbf{g} && \text{on } \Gamma_N, \\ \boldsymbol{\sigma} \cdot \mathbf{n} &= 0 && \text{on } \Gamma, \\ \boldsymbol{\sigma}_\tau \cdot \mathbf{u} + s|\mathbf{u} \cdot \boldsymbol{\tau}| &= 0, \quad -s \leq \boldsymbol{\sigma}_\tau \leq s && \text{on } \Gamma_C, \end{aligned} \tag{2.86}$$

where the normal and tangential components of the displacement $\mathbf{u}$ on the boundary Γ are denoted by $\mathbf{u}_n$ and $\mathbf{u}_\tau$, respectively. These components are defined as $\mathbf{u}_n = \mathbf{u} \cdot \mathbf{n}$ and $\mathbf{u}_\tau = \mathbf{u} - \mathbf{u}_n \mathbf{n}$.

The set of admissible displacements is given by:

$$\mathbf{V} := \left\{ \mathbf{v} \in H^1(\Omega)^2 : \mathbf{v} = 0 \text{ a.e. on } \Gamma_D, \mathbf{v} \cdot \mathbf{n} = 0 \text{ a.e. on } \Gamma_C \right\}.$$

We define the bilinear and linear forms $a : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{R}^2$ and $L : H^1(\Omega) \rightarrow \mathbb{R}^2$, respectively, as:

$$a(\mathbf{u}, \mathbf{v}) := \int_{\Omega} \mathbb{C} \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) \, dx, \quad L(\mathbf{v}) := \int_{\Gamma_N} \mathbf{g} \cdot \mathbf{v} \, ds.$$

The inequality constraints imposed on the potential contact zone Γ_C lead to the variational formulation associated with (2.86) being expressed as a variational inequality:

$$a(\mathbf{u}, \mathbf{v} - \mathbf{u}) + j_T(\mathbf{v}) - j_T(\mathbf{u}) \geq L(\mathbf{v} - \mathbf{u}), \quad \forall \mathbf{v} \in \mathbf{V}, \tag{2.87}$$

where the nonlinear functional $j_T : H^1(\Omega) \rightarrow \mathbb{R}^2$ is defined as:

$$j_T(\mathbf{v}) := \int_{\Gamma_C} s |\mathbf{v}_\tau| \, ds.$$

This problem can equivalently be reformulated as a minimization problem:

$$\inf_{\mathbf{v} \in \mathbf{V}} \left\{ I(\mathbf{v}) = \frac{1}{2}a(\mathbf{v}, \mathbf{v}) - L(\mathbf{v}) + j_T(\mathbf{v}) \right\}.$$

The solution $\mathbf{u} \in H^1(\Omega)$ of (2.86) satisfies:

$$I(\mathbf{u}) = \inf_{\mathbf{v} \in \mathbf{V}} I(\mathbf{v}). \quad (2.88)$$

The necessary and sufficient optimality conditions for (2.88) are expressed as:

$$a(\mathbf{u}, \mathbf{v} - \mathbf{u}) - L(\mathbf{v} - \mathbf{u}) + j_T(\mathbf{v}) - j_T(\mathbf{u}) \geq 0, \quad \mathbf{u} \in \mathbf{V}, \mathbf{v} \in \mathbf{V}. \quad (2.89)$$

To enable shape optimization for the elasticity problem involving frictional contact, one must overcome a significant challenge: the inherent non-smoothness of the frictional potential. The original friction term, modeled by the functional

$$j_T(\mathbf{u}_\tau) := \int_{\Gamma_C} s|\mathbf{u}_\tau| ds, \quad (2.90)$$

is non-differentiable due to the absolute value operator, which prevents the direct application of gradient-based optimization algorithms.

To address this difficulty, we employ a regularization strategy that smooths the non-differentiable friction potential while preserving its physical meaning. This technique has been developed and analyzed in the context of variational inequalities and contact mechanics (see, e.g., Chaudet-Dumas, 2023; Chaudet-Dumas and Deteix, 2020, 2021).

Let $\eta > 0$ be a small regularization parameter. We introduce a smoothing function $\theta(z, \eta)$ that approximates $|z|$ while being smooth (twice continuously Fréchet differentiable). It is defined as:

$$\theta(z, \eta) = \begin{cases} |z|, & \text{if } |z| > \eta, \\ \Lambda(\eta; z), & \text{if } |z| \leq \eta, \end{cases} \quad (2.91)$$

where the smoothing polynomial Λ is chosen such that θ is $\mathcal{C}^2$ and matches $|z|$ and its derivatives at the transition point $|z| = \eta$. A commonly used form is:

$$\Lambda(\eta; z) = -\frac{1}{8\eta^3}|z|^8 + \frac{3}{4\eta}|z|^4 + \frac{3\eta}{8}. \quad (2.92)$$

This construction ensures that $\theta(z, \eta) \approx |z|$ for small η while maintaining smoothness necessary for sensitivity analysis.

With this smoothing function, the regularized frictional potential becomes:

$$j_{T,\eta}(\mathbf{u}_\tau) := \int_{\Gamma_C} s\theta(\mathbf{u}_\tau, \eta) ds, \quad (2.93)$$

which is now twice Fréchet differentiable, as shown in Maury et al., 2017.

We now formulate the regularized variational problem that replaces the original variational inequality. Let $\mathbf{V}_1 := \{\mathbf{v} \in H^1(\Omega)^2 : \mathbf{v} = 0 \text{ on } \Gamma_D\}$, and note that tangential boundary conditions (e.g., $\mathbf{v} \cdot \mathbf{n} = 0$ on Γ_C) are naturally embedded via the definition of the tangential component $\mathbf{v}_\tau = \mathbf{v} - (\mathbf{v} \cdot \mathbf{n})\mathbf{n}$.

The regularized state equation then reads: Find $\mathbf{u}_\eta \in \mathbf{V}_1$ such that:

$$a(\mathbf{u}_\eta, \mathbf{v}) + \langle \partial j_{T,\eta}(\mathbf{u}_{\eta,\tau}), \mathbf{v}_\tau \rangle_{\Gamma_C} = L(\mathbf{v}), \quad \forall \mathbf{v} \in \mathbf{V}_1. \quad (2.94)$$

Here, $\partial j_{T,\eta}$ denotes the Fréchet derivative of the regularized potential, and $\langle \cdot, \cdot \rangle_{\Gamma_C}$ is the L^2 duality pairing on the contact boundary.

Let $\mathbf{g}$ be the boundary traction control applied on Γ_N . The objective is to choose $\mathbf{g}$ so as to minimize a quadratic tracking-type cost functional, which measures the misfit between the actual state $\mathbf{u}_\eta$ and a desired displacement field $\mathbf{u}_d$, as well as penalizes the control effort:

$$J(\mathbf{g}) := \frac{1}{2} \int_{\Omega} |\mathbf{u}_\eta - \mathbf{u}_d|^2 dx + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}|^2 ds, \quad (2.95)$$

where $\beta > 0$ is the regularization parameter that balances tracking fidelity and control sparsity.

To compute the gradient of J with respect to the shape or the control, we introduce the regularized adjoint state $\mathbf{p}_\eta \in \mathbf{V}_1$, which satisfies the following variational equation:

$$a(\mathbf{p}_\eta, \mathbf{v}) + \langle j''_{T,\eta}(\mathbf{u}_{\eta,\tau})\mathbf{p}_{\eta,\tau}, \mathbf{v}_\tau \rangle_{\Gamma_C} = - \int_{\Omega} (\mathbf{u}_\eta - \mathbf{u}_d) \cdot \mathbf{v}, \quad \forall \mathbf{v} \in \mathbf{V}_1. \quad (2.96)$$

Here, $j''_{T,\eta}$ denotes the second Fréchet derivative of the regularized potential with respect to the tangential component. This adjoint equation arises from differentiating the Lagrangian of the optimization problem and is essential for computing gradients with respect to $\mathbf{g}$ or the domain shape.

Having regularized the non-smooth frictional contact condition and established a differentiable framework for the shape optimization of the elastic system with friction, it is natural to extend the analysis to include topological variations of the domain. While shape derivatives measure sensitivity with respect to infinitesimal boundary deformations, topological derivatives evaluate the impact of introducing small inclusions

or voids inside the domain. This provides a powerful tool for material distribution and structural design, especially in the presence of contact and friction conditions. In the following, we perform a topological sensitivity analysis for the elastic control problem with frictional contact on Γ_C , focusing on the impact of introducing small holes or inhomogeneities in the interior of the domain Ω .

2.6.1 Topological sensitivity analysis of the elastic control problem with frictional contact

As previously introduced, let $\hat{x}$ be an arbitrary fixed point in the domain $\Omega \subset \mathbb{R}^d$, and let $\omega \subset \mathbb{R}^d$ be a given smooth domain, typically chosen as a ball or ellipsoid, centered at the origin. We define a singular perturbation of the reference domain by removing a small inclusion centered at $\hat{x}$. Specifically, we define the perturbed domain as:

$$\Omega_\varepsilon := \Omega \setminus \overline{\omega_\varepsilon}, \quad \text{where } \omega_\varepsilon := \hat{x} + \varepsilon\omega,$$

for some small $\varepsilon > 0$. The topological sensitivity analysis investigates the first-order variation of a cost functional when such an infinitesimal hole is introduced into the domain.

We now restate the optimality system for the regularized frictional contact control problem on the perturbed domain Ω_ε . The goal is to characterize how the removal of ω_ε affects the state, adjoint, and control fields. We assume all unknowns are well-defined on Ω_ε and consider the following system:

State Equation on Ω_ε : Find $\mathbf{u}_\varepsilon \in \mathbf{V}(\Omega_\varepsilon)$ such that for all $\mathbf{v} \in \mathbf{V}(\Omega_\varepsilon)$,

$$\int_{\Omega_\varepsilon} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon) : \mathbf{e}(\mathbf{v}) dx + \int_{\Gamma_C} \partial j_{T,\eta}(\mathbf{u}_{\tau,\varepsilon}) \cdot \mathbf{v}_\tau ds = \int_{\Gamma_N} \mathbf{g}_\varepsilon \cdot \mathbf{v} ds. \quad (2.97)$$

Adjoint Equation on Ω_ε : Find $\mathbf{p}_\varepsilon \in \mathbf{V}(\Omega_\varepsilon)$ such that for all $\boldsymbol{\psi} \in \mathbf{V}(\Omega_\varepsilon)$,

$$\int_{\Omega_\varepsilon} \boldsymbol{\sigma}(\mathbf{p}_\varepsilon) : \mathbf{e}(\boldsymbol{\psi}) dx + \int_{\Gamma_C} j''_{T,\eta}(\mathbf{u}_{\tau,\varepsilon}) \mathbf{p}_{\tau,\varepsilon} \cdot \boldsymbol{\psi}_\tau ds = - \int_{\Omega_\varepsilon} (\mathbf{u}_\varepsilon - \mathbf{u}_d) \cdot \boldsymbol{\psi} dx. \quad (2.98)$$

Optimality Condition: The optimal control $\mathbf{g}_\varepsilon$ satisfies:

$$\mathbf{g}_\varepsilon = -\frac{1}{\beta} \mathbf{p}_\varepsilon \quad \text{on } \Gamma_N. \quad (2.99)$$

We now define the cost functional in the perturbed domain Ω_ε as:

$$\mathcal{J}_\varepsilon(\Omega) := \inf_{\mathbf{h} \in L^2(\Gamma_N)^d} I_\varepsilon(\mathbf{h}) = I_\varepsilon(\mathbf{g}_\varepsilon), \quad (2.100)$$

where the control-to-state mapping $\mathbf{h} \mapsto \mathbf{u}_\varepsilon$ is implicitly defined by the regularized variational inequality.

Substituting the optimal state and control into the objective, the value of the shape functional in Ω_ε is given by:

$$\mathcal{J}_\varepsilon(\Omega) = \frac{1}{2} \int_{\Omega_\varepsilon} |\mathbf{u}_\varepsilon - \mathbf{u}_d|^2 dx + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}_\varepsilon|^2 ds. \quad (2.101)$$

This expression will serve as the starting point for deriving the topological derivative, which quantifies the leading-order change in $\mathcal{J}_\varepsilon$ as $\varepsilon \rightarrow 0$. In the following, we will analyze this variation rigorously by comparing solutions on Ω_ε and Ω , applying asymptotic expansions and adjoint-based sensitivity techniques.

We consider the state equation in Ω_R by $\mathcal{S}_\varepsilon$: Find $\mathbf{u}_\varepsilon^R \in \mathbf{V}(\Omega_R)$, such that for $\forall \mathbf{v} \in \mathbf{V}(\Omega_R)$,

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon^R) : \mathbf{e}(\mathbf{v}) + \langle \mathcal{S}_\varepsilon(\mathbf{u}_\varepsilon^R), \mathbf{v} \rangle_{\partial B_R} + \langle \partial j_{T,\eta}(\mathbf{u}_{\tau,\varepsilon}^R), \mathbf{v}_\tau \rangle_{\Gamma_C} = \langle \mathbf{g}_\varepsilon^R, \mathbf{v} \rangle_{\Gamma_N}, \quad (2.102)$$

and we denote

$$a(\Omega_R; \mathbf{u}_\varepsilon^R, \mathbf{v}) := \int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\varepsilon^R) : \mathbf{e}(\mathbf{v}) \quad (2.103)$$

Also, the adjoint equation in Ω_R by $\mathcal{S}_\varepsilon$: Find $\mathbf{p}_\varepsilon^R \in \mathbf{V}(\Omega_R)$, such that for $\forall \mathbf{v} \in \mathbf{V}(\Omega_R)$,

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{p}_\varepsilon^R) : \mathbf{e}(\mathbf{v}) + \langle \mathcal{S}_\varepsilon(\mathbf{p}_\varepsilon^R), \mathbf{v} \rangle_{\partial B_R} + \langle j_{T,\eta}''(\mathbf{u}_{\tau,\varepsilon}^R) \mathbf{p}_{\tau,\varepsilon}, \mathbf{v}_\tau \rangle_{\Gamma_C} = - \int_{\Omega} (\mathbf{u}_\varepsilon^R - \mathbf{u}_d) \cdot \mathbf{v}. \quad (2.104)$$

We consider the following ansätze for the solutions $\mathbf{u}_\varepsilon, \mathbf{p}_\varepsilon, \mathbf{g}_\varepsilon$ to the topologically perturbed coupled system:

$$\begin{aligned} \mathbf{u}_\varepsilon &= \mathbf{u} + \varepsilon^d \mathbf{u}_1 + \tilde{\mathbf{u}}_\varepsilon, \\ \mathbf{p}_\varepsilon &= \mathbf{p} + \varepsilon^d \mathbf{p}_1 + \tilde{\mathbf{p}}_\varepsilon, \\ \mathbf{g}_\varepsilon &= \mathbf{g} + \varepsilon^d \mathbf{g}_1 + \tilde{\mathbf{g}}_\varepsilon, \end{aligned} \quad (2.105)$$

where $\mathbf{u}, \mathbf{p}, \mathbf{g}$ are solutions to the unperturbed coupled system; $\mathbf{u}_1, \mathbf{p}_1, \mathbf{g}_1$ are the first-order asymptotic correction terms and $\tilde{\mathbf{u}}_\varepsilon, \tilde{\mathbf{p}}_\varepsilon, \tilde{\mathbf{g}}_\varepsilon$ are the remainders of order $o(\varepsilon^d)$.

We differentiate (2.102) with $\rho = \varepsilon^d$ at $\varepsilon = 0^+$,

$$a(\Omega_R; \mathbf{u}_1, \mathbf{v}) + \langle \mathcal{S}(\mathbf{u}_1), \mathbf{v} \rangle_{\partial B_R} + \langle \mathcal{S}_1(\mathbf{u}), \mathbf{v} \rangle_{\partial B_R} + \langle j_{T,\eta}''(\mathbf{u}_\tau) \mathbf{u}_{1,\tau}, \mathbf{v}_\tau \rangle_{\Gamma_C} = \langle \mathbf{g}_1, \mathbf{v} \rangle_{\Gamma_N}. \quad (2.106)$$

$$\mathbf{g}_1 = -\frac{1}{\beta} \mathbf{p}_1 \text{ on } \Gamma_N. \quad (2.107)$$

We have the shape functional

$$\mathcal{J}_\varepsilon(\hat{x}) = \frac{1}{2} \int_{\Omega_R} |\mathbf{u}_\varepsilon^R - \mathbf{u}_d|^2 + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}_\varepsilon^R|^2. \quad (2.108)$$

Then we differentiate (2.108) with $\rho = \varepsilon^d$ at $\varepsilon = 0^+$.

$$\mathcal{T}(\hat{x}) = \int_{\Omega_R} (\mathbf{u}^R - \mathbf{u}_d) \cdot \mathbf{u}_1 + \beta \int_{\Gamma_N} \mathbf{g}^R \cdot \mathbf{g}_1. \quad (2.109)$$

Now, let us rewrite the adjoint system as

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{p}) : \mathbf{e}(\mathbf{v}) + \int_{\partial B_R} \mathcal{S}(\mathbf{p}) \cdot \mathbf{v} + \int_{\Gamma_C} j''_{T,\eta}(\mathbf{u}_\tau) \mathbf{p}_\tau \mathbf{v}_\tau = - \int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{v}. \quad (2.110)$$

By taking $\mathbf{u}_1$ as the test functions in (2.110), we have the following equalities:

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{p}) : \mathbf{e}(\mathbf{u}_1) + \int_{\partial B_R} \mathcal{S}(\mathbf{p}) \cdot \mathbf{u}_1 + \int_{\Gamma_C} j''_{T,\eta}(\mathbf{u}_\tau) \mathbf{p}_\tau \mathbf{u}_{1,\tau} = - \int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{u}_1. \quad (2.111)$$

On the other hand, by taking $\mathbf{p}$ as the test functions in (2.106), we obtain

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_1) : \mathbf{e}(\mathbf{p}) + \int_{\partial B_R} (\mathcal{S}_1(\mathbf{u}) + \mathcal{S}(\mathbf{u}_1)) \cdot \mathbf{p} + \int_{\Gamma_C} j''_{T,\eta}(\mathbf{u}_\tau) \mathbf{u}_{1,\tau} \mathbf{p}_\tau = \int_{\Gamma_N} \mathbf{g}_1 \cdot \mathbf{p} = -\beta \int_{\Gamma_N} \mathbf{g}_1 \cdot \mathbf{g}. \quad (2.112)$$

Combining the above equalities yields the following important result:

$$\int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{u}_1 + \beta \int_{\Gamma_N} \mathbf{g}_1 \cdot \mathbf{g} = \int_{\partial B_R} \mathcal{S}(\mathbf{u}_1) \cdot \mathbf{p} = -\mathbb{P}_r \boldsymbol{\sigma}(\mathbf{u}) : \mathbf{e}(\mathbf{p}). \quad (2.113)$$

Then the topological derivative

$$\mathcal{T}(\hat{x}) = \int_{\Omega_R} (\mathbf{u} - \mathbf{u}_d) \cdot \mathbf{u}_1 + \beta \int_{\Gamma_N} \mathbf{g} \cdot \mathbf{g}_1 = -\mathbb{P}_r \boldsymbol{\sigma}(\mathbf{u}(\hat{x})) : \mathbf{e}(\mathbf{p}(\hat{x})). \quad (2.114)$$

2.7 Numerical experiments

2.7.1 Numerical examples based on shape gradient

In this section, we present a series of numerical experiments designed to validate the theoretical results and demonstrate the practical effectiveness of the proposed shape optimization framework. Our focus is on solving the shape optimization problem governed by linear elasticity with boundary control and, where applicable, frictional contact conditions. The goal is to minimize the given cost functional by iteratively updating the domain shape using shape derivatives.

To this end, we adopt the shape gradient descent method, which remains one of the most widely used algorithms in shape optimization due to its simplicity, ease of implementation, and compatibility with a variety of geometric representations (e.g., level-set methods, mesh deformation techniques). A critical component of this method is the choice of descent direction, which is determined by the shape gradient, that is, the Eulerian derivative of the cost functional with respect to domain perturbations.

However, the shape gradient obtained analytically, especially in the form of boundary integrals, is often not directly usable for numerical purposes due to its limited regularity or lack of extension into the full computational domain. To address this, we apply a Hilbertian regularization technique (see, e.g., Sokolowski and Zolesio, 1992) to convert the shape gradient into a smoother vector field suitable for domain deformation.

Concretely, we define the regularized descent direction $\mathcal{V} \in \mathbf{H}_0^1(\Omega)^d$ as the solution of the following elliptic variational problem:

$$(D\mathcal{V}, D\mathbf{W})_{L^2(\Omega)} + (\mathcal{V}, \mathbf{W})_{L^2(\Omega)} = -dJ(\Omega; \mathbf{W}) \quad \forall \mathbf{W} \in \mathbf{H}_0^1(\Omega)^d. \quad (2.115)$$

This equation can be interpreted as solving a Poisson-type problem with homogeneous Dirichlet boundary conditions, where the right-hand side is driven by the (negative) shape derivative evaluated in test directions. The inclusion of the L^2 inner product in both gradient and function space terms ensures coercivity and stabilizes the solution, while guaranteeing that the descent direction $\mathcal{V}$ is sufficiently smooth and tangentially continuous for mesh updates.

Once the descent direction $\mathcal{V}$ is computed, we perform a shape update using a geometric transformation $F_t(x) := x + t\mathcal{V}(x)$, where $t > 0$ is a step size chosen via an Armijo-type backtracking line search or fixed heuristic. The domain Ω is then updated accordingly, and the state, adjoint and optimality conditions systems are re-solved on the new domain in the next iteration.

Through this iterative procedure, the algorithm consistently moves the domain in directions that decrease the objective functional, ultimately converging to a locally optimal shape under the given model and regularization.

To effectively track evolving domain boundaries during shape optimization—particularly when large deformations or topological changes may occur—we employ the level-set method Osher and Fedkiw, 2006; Saye and Sethian, 2020, originally introduced by Osher and Sethian, 1988 for free boundary problems and later widely used in shape and topology optimization (cf. Allaire et al., 2004).

Let $\Omega(t) \subset \Omega$ denote the design subdomain at time t , implicitly represented by a

level-set function $\phi : \Omega \times [0, T] \rightarrow \mathbb{R}$ satisfying:

$$\begin{cases} \phi(t, x) < 0 \iff x \in \Omega(t), \\ \phi(t, x) > 0 \iff x \in D \setminus \overline{\Omega(t)}, \\ \phi(t, x) = 0 \iff x \in \Gamma(t). \end{cases} \quad (2.116)$$

This representation enables flexible shape evolution and facilitates numerical handling of complex topological transitions.

To evolve the domain shape, we advect the level-set function using a velocity field $\mathcal{V}(t, x)$ derived from the shape gradient. The evolution equation takes the following Hamilton–Jacobi form Osher and Sethian, 1988:

$$\begin{cases} \frac{\partial \phi}{\partial t}(t, x) + \mathcal{V}(t, x) \cdot \nabla \phi(t, x) = 0 & \text{in } \Omega \times (0, T), \\ \phi(0, x) = \phi_0(x) & \text{in } \Omega, \end{cases} \quad (2.117)$$

where ϕ_0 is the initial level-set function—typically chosen as the signed distance function, which satisfies $|\nabla \phi_0| = 1$ near the boundary to ensure good numerical behavior.

As ϕ evolves, it may lose its distance property, becoming too flat or steep near $\partial\Omega(t)$. To maintain numerical stability, we periodically reinitialize ϕ by solving the re-distancing equation:

$$\begin{cases} \frac{\partial \phi}{\partial \tau}(x) + \text{sgn}(\phi_0(x)) (|\nabla \phi(x)| - 1) = 0 & \text{in } \Omega \times (0, T), \\ \phi(0, x) = \phi_0(x) & \text{in } \Omega, \end{cases} \quad (2.118)$$

where τ is a fictitious time variable. This step ensures that ϕ maintains desirable geometric and numerical properties throughout the optimization process.

By combining the level-set representation with a steepest descent method, where the velocity field $\mathcal{V}$ is computed from the shape gradient (e.g., via Hilbertian regularization), we obtain a flexible and robust shape optimization framework. This method naturally accommodates changes in topology and geometry, and is especially well-suited for problems involving evolving or complex boundaries, such as those with contact or interface conditions.

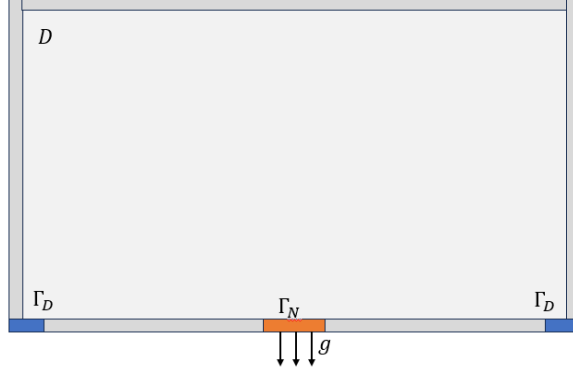


Figure 2.2: Schematic representation of the elastic domain.

Algorithm 1 Shape Steepest Descent Method

Require: Desired state $\mathbf{u}_d$, initial level-set function ϕ_0 , regularization parameters β

- 1: Set $k \leftarrow 0$
 - 2: **repeat**
 - 3: Solve the state equation
 - 4: Solve the adjoint equation
 - 5: Solve the optimality conditions
 - 6: Compute the descent direction $\mathcal{V}$ by solving the Hilbertian regularization equation
 - 7: Update the level-set function ϕ^k by solving the transport equation
 - 8: **if** reinitialization is needed **then**
 - 9: Reinitialize ϕ^k by solving the re-distancing equation
 - 10: **end if**
 - 11: $k \leftarrow k + 1$
 - 12: **until** $|J(\Omega^{k+1}) - J(\Omega^k)| < \epsilon |J(\Omega^k)|$
-

Example 2.7.1. We present a two-dimensional numerical experiment to demonstrate the effectiveness of the proposed topological optimization algorithm. The computational domain is a rectangle defined as $D = [0, 2] \times [0, 1]$, as illustrated in Fig. 2.2. Homogeneous Dirichlet boundary conditions are imposed at the bottom left and right ends, enforcing zero displacement. A vertical unit point load is applied at the midpoint of the bottom edge, which serves as the external forcing condition.

To define the target displacement field $\mathbf{u}_d$, we begin by solving the linear elasticity state system on the initial full domain without any voids. The resulting displacement

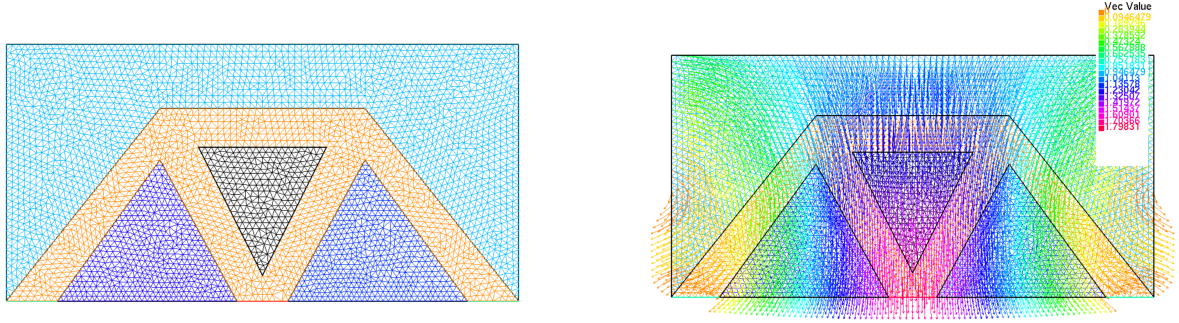


Figure 2.3: Desired structural configuration and target displacement field $\mathbf{u}_d$.

field is then used as the desired target in the optimization problem. The computed target displacement $\mathbf{u}_d$ is shown in Fig. 2.3.

The shape optimization process is performed using the algorithm 1 which employs a level set based domain representation. The level set method tracks the evolution of the structural domains, while the shape gradients provide sensitivity information indicating which directions minimize the objective function.

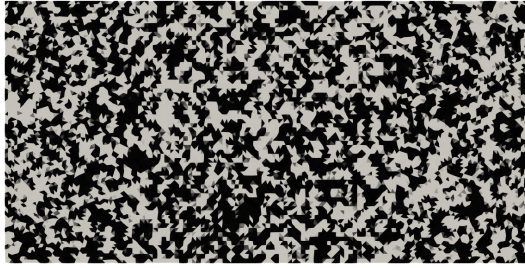
In our numerical simulations, we use the following material and physical parameters:

- Young's modulus: $E = 1.0$,
- Poisson's ratio: $\nu = 0.3$,

A volume constraint is incorporated into the optimization formulation using a Lagrange multiplier, which is set to $\ell = 25$ in this example. This constraint helps maintain a prescribed volume fraction of material during the optimization process.

After several iterations, the algorithm converges to an optimal structural topology, as shown in Fig. 2.4. The final design achieves a material layout that balances structural performance with minimal material usage while satisfying the boundary conditions and loading requirements.

The convergence behavior of the objective functional $J(\Omega)$ over the course of the iterations is depicted in Fig. 2.5. The optimization process minimizes the objective functional while simultaneously updating the control variable g . In this example, g gradually approaches the desired value $g^* = 1.0$, demonstrating stable convergence behavior (see Fig. 2.5).



(a) Initial shape



(b) Iteration 3



(c) Iteration 5



(d) Iteration 10



(e) Iteration 12



(f) Final shape

Figure 2.4: Shape evolution over optimization iterations.

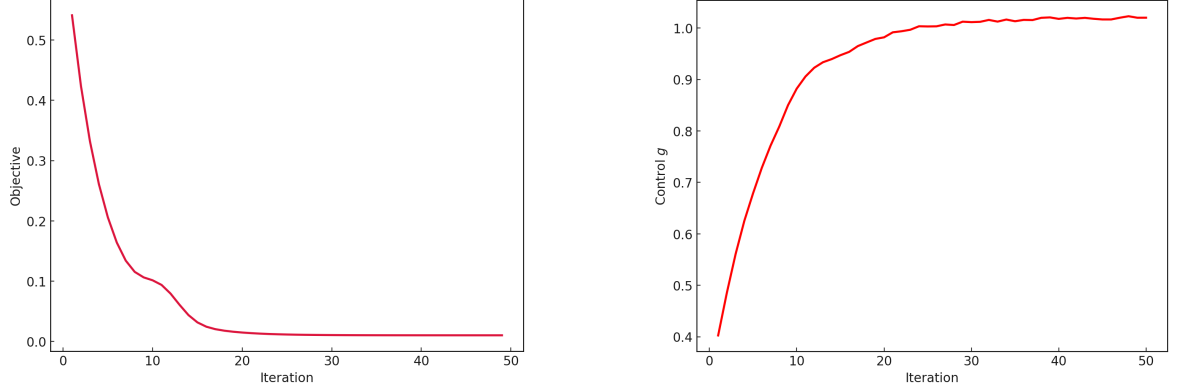


Figure 2.5: Convergence behavior of the objective functional and evolution of the control variable g during the optimization process.

2.7.2 Numerical examples based on topological derivative

Definition 2.7.1. Let $J : \mathcal{P}(D) \rightarrow \mathbb{R}$ be a shape functional, let $\Omega \in \mathcal{P}(D)$ be an open set, and let $\Gamma = \partial\Omega \setminus \partial D$. Assume that the topological derivative $\mathcal{T}(x)$ exists for all $x \in D \setminus \Gamma$. We define the generalized topological derivative as

$$\tilde{\mathcal{T}}(x) := \begin{cases} -\mathcal{T}(x) & \text{if } x \in \Omega, \\ \mathcal{T}(x) & \text{if } x \in D \setminus \bar{\Omega}. \end{cases} \quad (2.119)$$

Next, let $\phi : D \rightarrow \mathbb{R}$ be a level-set function representing the domain Ω . Suppose there exists a constant $c > 0$ such that

$$\tilde{\mathcal{T}}(x) = c\phi(x) \quad \text{for all } x \in D. \quad (2.120)$$

Under this condition, we obtain

$$\mathcal{T}(x) \geq 0 \quad \text{for all } x \in D \setminus \partial\Omega, \quad (2.121)$$

which constitutes a necessary condition for Ω to be optimal (cf. Amstutz and Andrä, 2006).

Following Amstutz and Andrä, 2006, we introduce a fictitious time t and consider a family of domains Ω_t , each represented by a level-set function $\phi : [0, T] \times D \rightarrow \mathbb{R}$. To derive a solution algorithm, the idea is to formulate an evolution equation for ϕ that ensures Ω_t converges to a minimizer as $t \rightarrow \infty$. A natural approach is to evolve the level-set function according to the generalized topological derivative $\tilde{\mathcal{T}}(\Omega_t)$:

$$\frac{\partial \phi(t, \cdot)}{\partial t} = P_{\phi_k^\perp} \left(\tilde{\mathcal{T}}(\Omega_k) \right), \quad t \geq 0, \quad (2.122)$$

where $P_{\phi_k^\perp}$ is the orthogonal projector onto the orthogonal complement of ϕ :

$$P_{\phi_k^\perp}(\tilde{\mathcal{T}}) = \tilde{\mathcal{T}} - \frac{(\tilde{\mathcal{T}}, \phi)}{\|\phi\|^2} \phi. \quad (2.123)$$

Here, $(\tilde{\mathcal{T}}, \phi) = (\tilde{\mathcal{T}}, \phi)_{L^2(\mathbb{D})}$ denotes the $L^2(\mathbb{D})$ -scalar product.

If the right-hand side of (2.122) vanishes, i.e., $P_{\phi_k^\perp}(\tilde{\mathcal{T}}(\Omega_k)) = 0$, then there exists some $\alpha \in \mathbb{R}$ such that $\tilde{\mathcal{T}}(\Omega_k) = \alpha\phi$. If $\alpha > 0$, then the necessary optimality conditions (2.121) are satisfied, and the geometry Ω described by ϕ is a local minimizer.

To quantify convergence, we may consider the norm of the projected topological derivative:

$$\left\| P_{\phi^\perp}(\tilde{\mathcal{T}}(\Omega)) \right\|_{L^2(\mathbb{D})}. \quad (2.124)$$

Another useful indicator is the angle

$$\theta_n = \arccos \left(\frac{(\phi_n, \tilde{\mathcal{T}}(\Omega_n))}{\|\phi_n\|_{L^2(\mathbb{D})} \|\tilde{\mathcal{T}}(\Omega_n)\|_{L^2(\mathbb{D})}} \right), \quad (2.125)$$

which, if sufficiently small, implies $P_{\phi^\perp}(\tilde{\mathcal{T}}(\Omega)) \approx 0$, thereby indicating that the necessary optimality conditions are approximately met.

To implement the algorithm, we discretize (2.122) using the explicit Euler method:

$$\frac{\phi_{n+1} - \phi_n}{\delta t} = P_{\phi_n^\perp}(\tilde{\mathcal{T}}(\Omega_n)) \quad \Leftrightarrow \quad \phi_{n+1} = \phi_n + \delta t P_{\phi_n^\perp}(\tilde{\mathcal{T}}(\Omega_n)), \quad (2.126)$$

where n denotes the current time step.

Rather than strictly considering $\delta t \rightarrow 0$ for a gradient flow approximation, we follow the interpretation in Blauth and Sturm, 2023 and treat (2.126) as a gradient descent method, where δt acts as a step size. This perspective allows us to leverage the convergence behavior of gradient descent and, when appropriate, employ larger step sizes to reduce computational effort.

In this framework, we interpret:

$$g_n = -P_{\phi_n^\perp}(\tilde{\mathcal{T}}(\Omega_n)) \quad (2.127)$$

as the “gradient” associated with the topology optimization problem. The full optimization procedure is outlined in Algorithm 2

Algorithm 2 Combined Level set function and Topological Derivative Optimization

Require: Initial level-set function ϕ_0 , initial step sizes t_0 , stopping tolerance $\text{Tol} > 0$, maximum number of iterations $n_{\max} \in \mathbb{N}$

- 1: Set $n \leftarrow 0$
- 2: **repeat**
- 3: Solve the state equation
- 4: Solve the adjoint equation
- 5: Solve the Optimality Condition
- 6: Compute the topological derivative $\bar{\mathcal{T}}(\Omega_n)$
- 7: Compute projected descent direction:

$$g_n = -P_{\phi_n}(\tilde{\mathcal{T}}(\Omega_n)) = -\left(\tilde{\mathcal{T}}(\Omega_n) - \frac{(\tilde{\mathcal{T}}(\Omega_n), \phi_n)}{\|\phi_n\|_{L^2(\mathcal{D})}^2} \phi_n\right)$$

- 8: Update the level-set function: $\phi_{n+1} = \phi_n - \tau_n g_n$
 - 9: **while** $J_\lambda(\phi_{n+1}) > J_\lambda(\phi_n)$ **do**
 - 10: Reduce the step size: $\tau_n \leftarrow \tau_n/2$
 - 11: **end while**
 - 12: Update the domain: $\Omega_{n+1} \leftarrow \Omega_n - t_n \theta_n$
 - 13: $n \leftarrow n + 1$
 - 14: **until** $|J_\lambda(\Omega_{n+1}) - J_\lambda(\Omega_n)| < \text{Tol} \cdot |J_\lambda(\Omega_n)|$
-

Example 2.7.2. *In this numerical example, we investigate a shape optimization problem for a linear elasticity control system with frictional contact boundary conditions. The model considers a two-dimensional rectangular structure as shown in Fig. 2.6. A homogeneous Dirichlet boundary condition is applied along the left boundary, meaning that the structure is fully fixed there with zero displacement. Meanwhile, a unit vertical pointwise load is applied at the midpoint of the right boundary to stimulate the structural response.*

The bottom boundary of the structure is designated as a potential frictional contact boundary, denoted by Γ_C . On this boundary, normal penetration is not allowed and certain friction laws are assumed to be satisfied. To handle the non-smoothness associated with friction, a regularized frictional potential is adopted, and the contact interaction is modeled within a variational inequality framework.

We begin with an initial shape, illustrated in Fig. 2.7. The linear elasticity state equation is then solved for this shape to obtain the displacement field $\mathbf{u}$ under the applied

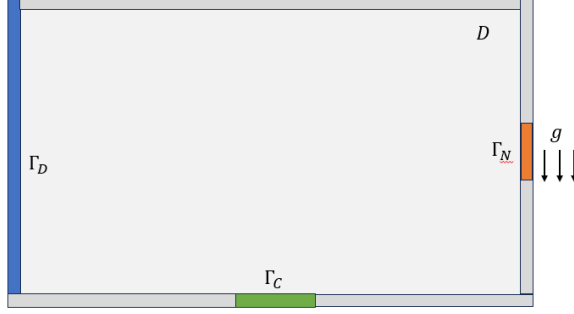


Figure 2.6: Schematic representation of the elastic contact domain.

load and boundary conditions. This displacement field serves as the target displacement u_d for the control objective.

To accurately control the structural response, we introduce a boundary control variable $\mathbf{g}$ and formulate the following objective functional:

$$J(\Omega) = \frac{1}{2} \int_{\Omega} |\mathbf{u} - \mathbf{u}_d|^2 dx + \frac{\beta}{2} \int_{\Gamma_N} |\mathbf{g}|^2 ds, \quad (2.128)$$

where β is a regularization parameter. By applying variational techniques, we derive the associated optimality system, which includes the state equation, the adjoint equation, and an explicit expression for the optimal control.

During the optimization process, we employ a topology-based structural optimization algorithm that utilizes the concept of topological derivatives in conjunction with the level-set method to track the evolution of the structural boundary. The frictional contact boundary condition is handled via a regularized potential to ensure differentiability of the state with respect to the shape.

We set the Lagrange multiplier $\ell = 20$ to impose a volume constraint. After several iterations, the optimized structure is obtained, as shown in Fig. 2.8. The results show that the optimized shape not only satisfies the frictional contact condition and the boundary control objectives but also exhibits improved geometry and stress transmission, demonstrating the effectiveness of the proposed optimization algorithm.

To further validate convergence, we plot the evolution of the objective functional $J(\Omega)$ over the iterations in Fig. 2.9. In this example, g gradually approaches but is not exactly equal to the expected value $g^* = 1.0$, exhibiting stable convergence behavior (see Figure 2.9).

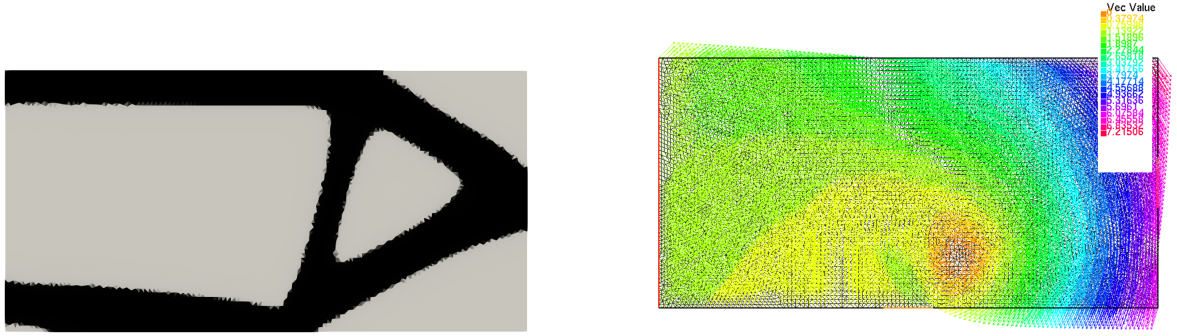
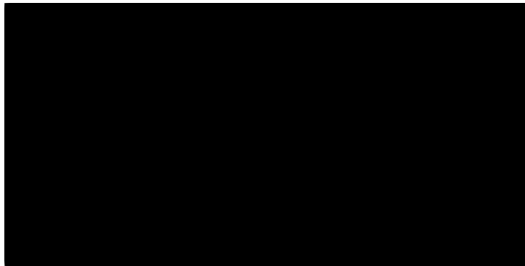
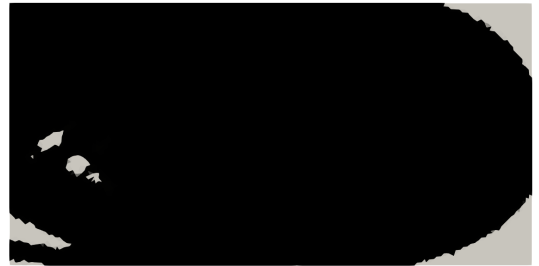


Figure 2.7: Desired structural configuration and target displacement field $\mathbf{u}_d$



(a) Initial shape



(b) Iteration 10



(c) Iteration 50



(d) Final Shape

Figure 2.8: Shape evolution over optimization iterations.

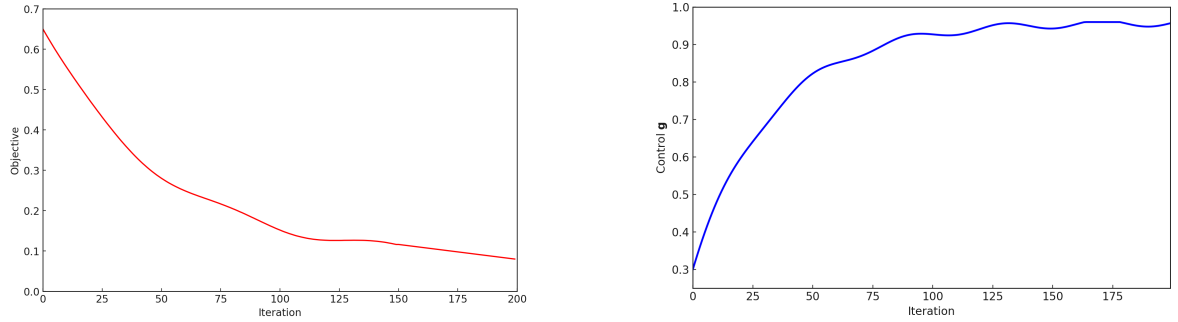


Figure 2.9: Convergence behavior of the objective functional and evolution of the control variable g during the optimization process.

2.8 From static to dynamic control - leveraging the turnpike property in linear elasticity

In the preceding chapters, we have developed a comprehensive framework for the optimal control of static linear elastic systems, including the modeling of the state and adjoint equations, the derivation of optimality conditions under frictional contact boundary conditions, and the implementation of shape and topology optimization strategies. These results not only provide deep insights into the design of elastic structures under steady loading but also lay the groundwork for extending the analysis to more complex dynamic scenarios.

In many real-world applications, however, elastic structures are subject to time-dependent loading or control actions, necessitating a dynamic formulation of the governing equations. In such cases, the system behavior becomes inherently time-dependent, and the corresponding optimal control problem is governed by hyperbolic or parabolic partial differential equations, significantly increasing the computational complexity.

A key insight from recent control theory—the turnpike property—offers a promising perspective for simplifying these dynamic problems. The turnpike phenomenon asserts that, under appropriate conditions, the optimal state and control remain close to their steady-state counterparts for the majority of the time horizon, deviating only near the initial and final time intervals. This implies that the solution to a time-dependent control problem can be well approximated by the corresponding steady-state control, especially when the time horizon is large.

In this context, we now shift our focus from static to dynamic control problems in linear elasticity and investigate how the turnpike property can be leveraged. This

not only enhances our theoretical understanding of the temporal structure of optimal solutions but also paves the way for computationally efficient algorithms by reducing dynamic control to steady-state optimization.

Building upon the preceding analysis of static optimal control problems in linear elasticity, we now explore how these insights extend to the time-dependent (dynamic) setting. In many structural optimization scenarios, time-dependent forces or responses cannot be neglected, especially in applications involving transient loads, vibrations, or wave propagation. However, solving time-dependent control problems can be computationally expensive due to the need to resolve fine time scales over long horizons.

This is where the turnpike property plays a central role. It states that for a broad class of optimal control problems governed by time-dependent partial differential equations (PDEs), the optimal state and control remain exponentially close to their steady-state counterparts over most of the time interval. Only near the initial and terminal time does the system significantly deviate from the steady configuration.

This phenomenon enables an efficient reduction of dynamic optimization to a static problem. For instance, the optimal control and displacement field in a dynamic elastic system can, under appropriate conditions, be approximated by those obtained from the corresponding steady-state problem. This not only reduces computational complexity but also provides qualitative insight into the long-term behavior of the system.

To make this idea precise, we formulate the dynamic elastic control problem, introduce a cost functional incorporating both displacement tracking and control effort, and derive the corresponding optimality system using a Lagrangian framework. The adjoint system now involves a time-reversed PDE, and the optimal control expression becomes time-dependent. If the turnpike property holds, the steady-state solution offers an accurate approximation, which we can utilize for efficient topology or shape optimization.

Furthermore, this approximation paves the way for applying static optimization techniques—such as shape gradients and topological derivatives—within a dynamic context. For example, one can design an optimized shape for a structure under dynamic loading by solving a steady control problem and leveraging its optimal topology as a surrogate for the time-dependent setting.

In what follows, we will formalize the dynamic optimal control problem, derive the associated optimality system, and discuss how the turnpike property connects this formulation with the steady-state case previously studied. We also highlight recent theoretical results that justify this reduction and demonstrate how it can be integrated

into numerical optimization algorithms.

2.8.1 Dynamic control problems

Building on the understanding of the steady-state control problem in linear elasticity, we now turn our attention to its dynamic counterpart. Dynamic control problems arise naturally in many engineering applications where the system evolves over time under external excitations or time-dependent boundary conditions. The modeling of such problems typically involves hyperbolic partial differential equations, notably the elastodynamic (wave-type) equation governed by the principles of momentum conservation.

We consider the time-dependent elastic system governed by the following strong form of the initial-boundary value problem:

$$\begin{aligned} \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot \boldsymbol{\sigma}(\mathbf{u}) &= \mathbf{f}(\mathbf{x}, t) \quad \text{in } \Omega \times (0, T), \\ \mathbf{u} &= \mathbf{0} \quad \text{on } \Gamma_D \times (0, T), \\ \boldsymbol{\sigma}(\mathbf{u})\mathbf{n} &= \mathbf{g}(\mathbf{x}, t) \quad \text{on } \Gamma_N \times (0, T), \\ \boldsymbol{\sigma}(\mathbf{u})\mathbf{n} &= \mathbf{0} \quad \text{on } \Gamma \times (0, T), \\ \mathbf{u}(\mathbf{x}, 0) &= \mathbf{u}_0(\mathbf{x}), \quad \frac{\partial \mathbf{u}}{\partial t}(\mathbf{x}, 0) = \mathbf{v}_0(\mathbf{x}) \quad \text{in } \Omega, \end{aligned} \tag{2.129}$$

where ρ is the mass density, $\boldsymbol{\sigma}(\mathbf{u})$ is the Cauchy stress tensor determined by the linear elasticity law, and $\mathbf{f}$ is a body force that may depend on time. The dynamic response $\mathbf{u}(\mathbf{x}, t)$ of the system is subject to initial conditions and boundary inputs.

The control objective, in analogy to the steady-state case, is to drive the displacement $\mathbf{u}$ to a desired trajectory $\mathbf{u}_d$ over the entire time interval $(0, T)$. We define the cost functional:

$$J(\mathbf{g}) = \frac{1}{2} \int_0^T \int_{\Omega} |\mathbf{u} - \mathbf{u}_d|^2 dx dt + \frac{\gamma}{2} \int_0^T \int_{\Omega} |\partial_t \mathbf{u}|^2 dx dt + \frac{\beta}{2} \int_0^T \int_{\Gamma_N} |\mathbf{g}|^2 ds dt, \tag{2.130}$$

where the second term penalizes high kinetic energy and the third term regularizes the control input $\mathbf{g}$. The parameter γ can be tuned to adjust the sensitivity of the functional to dynamic oscillations.

To derive the first-order optimality conditions, we introduce a time-dependent Lagrangian and deduce the adjoint system, which must be solved backward in time. This system includes the adjoint wave equation, along with corresponding boundary and terminal conditions.

Importantly, assuming the turnpike property holds, we expect that both the state and the control remain close to their optimal steady-state counterparts for most of the time interval, simplifying both analysis and computation. This opens the door to efficient approximations, where steady-state solutions provide useful initialization or guidance for solving the time-dependent problem.

To derive the first-order optimality conditions for the dynamic control problem governed by linear elasticity, we introduce an adjoint variable $\mathbf{p}(x, t)$ and construct a time-dependent Lagrangian functional:

$$\begin{aligned} \mathcal{L}(\mathbf{u}, \mathbf{g}, \mathbf{p}) = & \frac{1}{2} \int_0^T \int_{\Omega} |\mathbf{u} - \mathbf{u}_d|^2 dx dt + \frac{\gamma}{2} \int_0^T \int_{\Omega} |\partial_t \mathbf{u}|^2 dx dt + \frac{\beta}{2} \int_0^T \int_{\Gamma_N} |\mathbf{g}|^2 ds dt \\ & - \int_0^T \int_{\Omega} (\rho \partial_{tt} \mathbf{u} - \nabla \cdot \boldsymbol{\sigma}(\mathbf{u})) \cdot \mathbf{p} dx dt - \int_0^T \int_{\Gamma_N} (\boldsymbol{\sigma}(\mathbf{u}) \cdot \mathbf{n} - \mathbf{g}) \cdot \mathbf{p} ds dt. \end{aligned} \quad (2.131)$$

Here, $\mathbf{u}$ denotes the system displacement, $\mathbf{g}$ is the control, $\mathbf{u}_d$ is the desired displacement, and γ, β are regularization parameters. To derive the adjoint equation, we take the first variation of $\mathcal{L}$ with respect to the state variable $\mathbf{u}$, and apply integration by parts. This yields:

$$\delta_{\mathbf{u}} \mathcal{L} = \int_0^T \int_{\Omega} [(\mathbf{u} - \mathbf{u}_d) - \rho \partial_{tt} \mathbf{p} + \nabla \cdot \boldsymbol{\sigma}(\mathbf{p}) - \gamma \partial_{tt} \mathbf{u}] \cdot \delta \mathbf{u} dx dt. \quad (2.132)$$

Hence, the adjoint system satisfies the following equations:

$$\begin{aligned} \rho \partial_{tt} \mathbf{p} - \nabla \cdot \boldsymbol{\sigma}(\mathbf{p}) &= -(\mathbf{u} - \mathbf{u}_d) + \gamma \partial_{tt} \mathbf{u}, & \text{in } \Omega \times (0, T), \\ \mathbf{p} &= 0, & \text{on } \Gamma_D, \\ \boldsymbol{\sigma}(\mathbf{p}) \cdot \mathbf{n} &= 0, & \text{on } \Gamma_N \cup \Gamma, \\ \mathbf{p}(x, T) &= 0, \quad \partial_t \mathbf{p}(x, T) = 0, & \text{in } \Omega. \end{aligned} \quad (2.133)$$

To derive the optimal control expression, we consider the variation of $\mathcal{L}$ with respect to the control $\mathbf{g}$, yielding:

$$\delta_{\mathbf{g}} \mathcal{L} = \int_0^T \int_{\Gamma_N} (\beta \mathbf{g} + \mathbf{p}) \cdot \delta \mathbf{g} ds dt, \quad (2.134)$$

which leads to the optimality condition:

$$\mathbf{g}(x, t) = -\frac{1}{\beta} \mathbf{p}(x, t), \quad \text{on } \Gamma_N. \quad (2.135)$$

Assuming that the Turnpike property Gugat and Sokolowski, 2023; Gugat et al., 2024 occurs for the optimality system, then we can directly optimize the static problem to design the dynamic problem.

The turnpike property indicates that, under certain conditions, the solutions of dynamic control problems stay close to their steady-state counterparts for the majority of the time horizon, with deviations occurring only near the initial and terminal times. This property significantly simplifies the computational process by allowing the dynamic control problem to be effectively approximated using steady-state optimization. The corresponding static problem for the dynamic system is governed by an elliptic state equation, enabling a dynamic-to-steady reduction. By leveraging the turnpike property, dynamic control problems can be addressed efficiently through steady-state formulations, greatly reducing the computational complexity while maintaining accuracy.

We obtain the numerical results for topology optimization of control problems governed by the linearized elasticity equation. The steady-state problems are considered as well as for control with given friction nonlinear boundary conditions. The shape functional is defined by the optimal cost of the control problems. The topological derivative method is applied to determine the optimal shape and topology of the integration domain for the elastic body with given reactions resulting from optimal control problem. In the paper the topological derivative method is applied to the solution of topology optimization problems for linear elasticity. The shape functional is given by the optimality system for a control problem. In the case of linear elasticity, the cost for the control problem is a tracking type functional. In the case of a contact problem with given friction the standard compliance functional is considered.

Assuming the turnpike property for a control problem under considerations the numerical method of shape design can be substantially simplified. The general proof of turnpike property is given in the paper Gugat and Sokolowski, 2023. The proof can be adopted to the case of control problems for elasticity systems in two spatial dimensions by an appropriate selection of the cost functional. In the case of linear elasticity, the tracking type functional is considered with the new component depending on the velocity u_t . In the case of a contact problem, the work functional with the same component depending on velocity can be considered. The application of the results obtained for the steady-state model are useful for the dynamic control and topology optimization provided the so-called Turnpike property Gugat and Sokolowski, 2023; Gugat et al., 2024 occurs for the dynamic control problem. In our setting, the control problem replaces the multi-load analysis of optimum design of the elastic structure. The tractions for control problems considered are selected taking into account a tracking type cost or the compliance of the structure.

Topology optimization for steady state problems is performed by the topological derivative method. The singular perturbations of geometrical domains are used for elliptic boundary value problems. The extension of the topological derivative method for the wave equation. Therefore we propose two optimal control problems for dynamical models which could be reduced, under the same assumptions to the steady state control problems.

The approximation of the wave equation for numerical methods can be approached in two main ways. One method involves finite element (FE) discretization, which transforms the problem into a second-order system of ordinary differential equations (ODEs) with respect to the time variable, as discussed in Chen, Wei, et al., 2023. Another approach employs finite difference approximations for time derivatives, effectively converting the wave equation into a sequence of elliptic problems. These numerical techniques facilitate efficient computation and analysis, and the Turnpike property for the discretized state equation can be demonstrated based on established theoretical results.

Chapter 3

Modeling and Simulation of Contact Problem via Phase Field Methods in Linear Elasticity

In the previous chapter, we systematically studied the control optimization problem in linear elasticity with frictional contact boundary conditions. By employing the level set method based on shape derivatives and topological derivatives, we successfully achieved the joint fulfillment of structural geometry optimization and control objectives. While this method demonstrates strong geometric expressiveness in handling boundary evolution and contact behavior, practical problems often involve contact boundaries with high uncertainty and nonsmooth characteristics. This is particularly challenging when the location of the contact zone is unknown or undergoes frequent changes, rendering traditional interface-tracking methods less effective.

To overcome these difficulties and enhance the modeling flexibility and numerical robustness for contact behavior, the next chapter introduces the phase-field method as a novel variational modeling framework for contact problems. The phase-field approach characterizes the distribution and evolution of interfaces by introducing an auxiliary variable that varies continuously between -1 and 1 , thereby eliminating the need for an explicitly represented contact boundary. This makes it naturally suited for handling complex contact phenomena such as nonsmoothness, irregular evolution, and even fracture. In the forthcoming analysis, we will focus on frictional contact problems in linear elasticity, construct the corresponding phase-field variational model, and investigate key aspects such as existence, regularization techniques, and numerical solution methods.

3.1 Contact problems in linearized elasticity

In solid mechanics and engineering science, contact problems Khludnev and Sokolowski, 1999; Maury et al., 2017 refer to the modeling and analysis of interactions between two or more bodies that come into contact with each other. These problems are ubiquitous in real-world applications such as mechanical assembly, bridge supports, gear engagement, crack closure, biological joint motion, and many others. Due to the fact that the contact status between bodies can change dynamically depending on external forces and structural deformations, contact problems are inherently nonlinear and non-deterministic, making them among the most challenging problems in computational mechanics.

When the deformation of the structure is relatively small, the theory of linearized elasticity is often used to describe the mechanical behavior of the material. This theory is based on small-strain assumptions and Hooke's law, which simplifies the governing equations while still capturing the essential physical responses of the system. Within this framework, the relationship between stress and strain is linear, and the internal stress state of the structure can be determined by solving a system of linear partial differential equations. However, the introduction of contact constraints fundamentally changes the nature of the problem. Instead of dealing solely with well-posed boundary value problems, one must now handle inequality constraints and complementarity conditions on the boundary, which leads to nonlinear formulations even in the context of linear material laws.

To set up a rigorous model, let us consider an elastic body occupying a bounded open domain $\Omega \subset \mathbb{R}^d$ with $d = 2$ or 3 . The boundary of the domain, $\partial\Omega$, is partitioned into several disjoint parts, each corresponding to a specific type of physical behavior: Γ_D denotes the clamped or fixed boundary where the displacement is prescribed to be zero; Γ_N is the part of the boundary where external loads are applied; Γ represents the free boundary, where neither traction nor displacement is prescribed; Γ_C represents a potential contact with a rigid obstacle; and S denotes an internal contact surface, modeling possible self-contact such as may occur along a fold, wrinkle, or closed crack surface. This partitioning is not only physically meaningful but also essential for formulating the problem mathematically.

In linear elasticity, the internal stress of the body is derived from the strain tensor, given by the symmetric part of the displacement gradient:

$$\varepsilon(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T).$$

The stress tensor $\boldsymbol{\sigma}$ is related to the strain via Hooke's law. For isotropic linear elastic materials, the relationship is typically written as:

$$\boldsymbol{\sigma} = A\boldsymbol{\varepsilon}(\mathbf{u}) = 2\mu\boldsymbol{\varepsilon}(\mathbf{u}) + \lambda \operatorname{tr}(\boldsymbol{\varepsilon}(\mathbf{u}))I, \quad (3.1)$$

where μ and λ are the Lamé parameters characterizing the material's shear and volumetric stiffness, respectively, and I is the identity tensor.

Without contact conditions, the equilibrium of the structure under body forces f and surface forces g leads to a classical linear boundary value problem. However, contact introduces additional unknowns—namely, the regions where contact actually occurs—which transforms the problem into a free boundary problem. In particular, on the contact boundary Γ_C , the body is not allowed to penetrate the obstacle, which translates into a non-penetration condition in the normal direction: $\mathbf{u}_n \leq 0$, where $\mathbf{u}_n = \mathbf{u} \cdot \mathbf{n}$ is the displacement in the normal direction. Moreover, contact pressure must be compressive (no adhesive force), implying: $\boldsymbol{\sigma}_n = (A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n}) \cdot \mathbf{n} \leq 0$. These two conditions are further coupled by the complementarity condition: $\mathbf{u}_n \cdot \boldsymbol{\sigma}_n = 0$. Together, these three constraints form the Signorini conditions, which are fundamental to modeling frictionless contact between an elastic body and a rigid obstacle.

For self-contact problems, such as those involving crack closure or surface folding, the mathematical model must account for the possibility that different parts of the same body may come into contact. In such cases, the internal contact surface S lies within the domain $\bar{\Omega}$, and one must define the jump in displacement across this surface: $[u] = u|_{S_-} - u|_{S_+}$, where S_- and S_+ denote the two opposing sides of the contact surface. The contact constraints are then formulated analogously to the Signorini conditions, but now applied to the jump $[u]_n$ and the sum of normal stresses on both sides of the interface.

From a mathematical standpoint, contact problems are variational inequalities (VIs) rather than classical boundary value problems. This is because the presence of inequality and complementarity constraints on the contact boundary precludes the use of standard variational (energy minimization) principles. Instead, one defines a convex admissible set K of feasible displacements that satisfy the unilateral contact conditions (e.g., $\mathbf{u}_n \leq 0$ on Γ_C), and seeks a displacement $\mathbf{u} \in K$ such that:

$$a(\mathbf{u}, \mathbf{v} - \mathbf{u}) \geq L(\mathbf{v} - \mathbf{u}), \quad \forall \mathbf{v} \in K, \quad (3.2)$$

where $a(\cdot, \cdot)$ is a bilinear form representing the internal elastic energy, and $L(\cdot)$ is the linear form corresponding to external forces. This variational inequality formulation

provides a solid theoretical foundation for both analytical and numerical treatment of contact problems.

Even though the material model is linear, the contact boundary conditions introduce nonlinearities, making the overall problem significantly more complex. A wide range of numerical techniques have been developed to handle such problems. The penalty method approximates the inequality constraints by adding a penalization term that enforces the constraint softly, at the cost of introducing a penalty parameter and possible ill-conditioning. The Lagrange multiplier method introduces additional unknowns to enforce the contact conditions exactly, leading to a saddle-point problem. The active set strategy, inspired by optimization theory, iteratively identifies the regions where contact occurs and solves the corresponding reduced problem, often yielding robust and efficient solvers.

In summary, contact models in linearised elasticity arise naturally in the modeling of mechanical systems where bodies interact through contact, whether with external obstacles or self-contact surfaces. Although the governing equations of linear elasticity are themselves linear, the incorporation of contact conditions transforms the problem into a highly nonlinear and constrained system. Accurately modeling and solving such systems requires a blend of physical insight, mathematical rigor, and numerical innovation. As such, contact modeling remains a crucial area in computational mechanics and continues to be an active field of research, particularly in the context of structural optimization, multi-body dynamics, and fracture mechanics.

Among the many models in contact mechanics, the Signorini problem is one of the most fundamental and classical. It describes the interaction between an elastic body and a rigid, impenetrable obstacle under the influence of external forces. Owing to its simplicity in physical modeling, precision in mathematical structure, and wide applicability in both engineering and numerical analysis, the Signorini problem has become a central subject in the study of frictionless contact mechanics. Compared with the sliding contact model, the Signorini problem is more abstract and focuses solely on the normal (perpendicular) contact behavior between a structure and an obstacle. It imposes no control over the tangential behavior, such as friction or slip, and hence serves both as a theoretical foundation and a generalization of more detailed frictionless contact models.

In this section, we present the formulation of the Signorini problem based on the previously defined linear elastic framework. We will explore its mathematical formulation, variational inequality representation, the nature of the free boundary, and its

significance in both theory and applications.

The physical scenario behind the Signorini problem is as follows: an elastic structure, occupying a domain Ω , is placed above or next to a rigid obstacle. When subjected to external forces, the structure may come into contact with the obstacle, or it may remain separated. Crucially, the contact region is not known a priori—it emerges as part of the solution. This characteristic distinguishes the problem from classical boundary value problems and classifies it as a free boundary problem.

From a mathematical standpoint, the Signorini problem is not a standard boundary value problem. Instead, it is a nonlinear problem with inequality constraints on the boundary. To treat this rigorously, it is formulated as a variational inequality.

Let $H_{\Gamma_D}^1(\Omega)^d$ denote the Sobolev space of vector-valued functions that vanish on the clamped part of the boundary Γ_D . We define the admissible set:

$$K := \{\mathbf{v} \in H_{\Gamma_D}^1(\Omega)^d \mid \mathbf{v} = 0 \text{ on } \Gamma_D, \text{ and } \mathbf{v} \cdot \mathbf{n} \leq 0 \text{ on } \Gamma_C\}, \quad (3.3)$$

which includes all displacements that satisfy the non-penetration condition.

Let us define the bilinear form:

$$a(\mathbf{u}, \mathbf{v}) := \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) \, dx, \quad (3.4)$$

and the linear functional:

$$L(\mathbf{v}) := \int_{\Omega} \mathbf{f} \cdot \mathbf{v} \, dx + \int_{\Gamma_N} P \cdot \mathbf{v} \, ds, \quad (3.5)$$

where $\mathbf{f}$ and P are the given volume and boundary forces, respectively.

Then the variational formulation of the Signorini problem reads: Find $\mathbf{u} \in K$ such that

$$a(\mathbf{u}, \mathbf{v} - \mathbf{u}) \geq L(\mathbf{v} - \mathbf{u}), \quad \forall \mathbf{v} \in K. \quad (3.6)$$

This inequality states that among all admissible displacements, the solution $\mathbf{u}$ is such that the energy cannot be further reduced by any other permissible displacement. In other words, $\mathbf{u}$ is a minimizer of the total potential energy over the feasible set K . Formally, this can be written as:

$$\mathbf{u} = \operatorname{argmin}_{\mathbf{v} \in K} \left[\frac{1}{2} \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{v}) : \boldsymbol{\varepsilon}(\mathbf{v}) \, dx - \int_{\Omega} \mathbf{f} \cdot \mathbf{v} \, dx - \int_{\Gamma_N} P \cdot \mathbf{v} \, ds \right]. \quad (3.7)$$

This constrained energy minimization problem is fundamental to both the analysis and numerical solution of the Signorini problem. Under standard assumptions (e.g., coercivity of $a(\cdot, \cdot)$ and continuity of $L(\cdot)$), the existence and uniqueness of the solution are guaranteed.

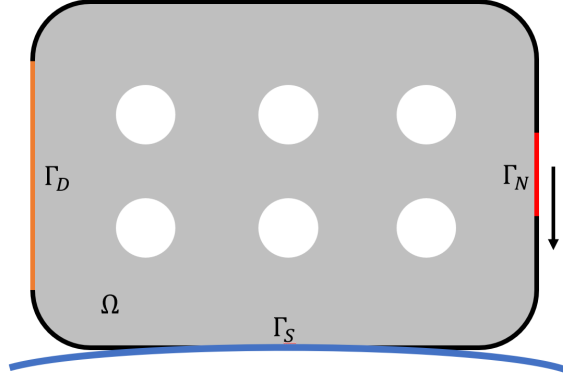


Figure 3.1: Schematic diagram of the Signorini problem model

3.2 Signorini contact problem

For a given body force $f \in C^\infty(\bar{\Omega})^d$, we consider the following Signorini problem in the framework of linearised elasticity, under the convention that the unit normal vector n is oriented outward from the domain:

$$\left\{ \begin{array}{ll} -\operatorname{div}(A\boldsymbol{\varepsilon}(\mathbf{u})) = f & \text{in } \Omega, \\ \mathbf{u} = 0 & \text{on } \Gamma_D, \\ A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n} = 0 & \text{on } \Gamma, \\ A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n} = P & \text{on } \Gamma_N, \\ \mathbf{u} \cdot \mathbf{n} \leq 0, \quad (A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n}) \cdot \mathbf{n} \leq 0, \quad (\mathbf{u} \cdot \mathbf{n})(A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n}) \cdot \mathbf{n} = 0 & \text{on } \Gamma_C. \end{array} \right. \quad (3.8)$$

Here, $\Omega \subset \mathbb{R}^2$ represents the reference configuration of a two-dimensional elastic body. The displacement field $\mathbf{u} : \Omega \rightarrow \mathbb{R}^2$ describes the deformation of the structure. The strain tensor is defined as

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T), \quad (3.9)$$

and the stress tensor $\boldsymbol{\sigma}(\mathbf{u}) = A\boldsymbol{\varepsilon}(\mathbf{u})$ satisfies Hooke's law for linear isotropic elasticity:

$$A\boldsymbol{\varepsilon}(\mathbf{u}) = 2\mu\boldsymbol{\varepsilon}(\mathbf{u}) + \lambda \operatorname{tr}(\boldsymbol{\varepsilon}(\mathbf{u}))I, \quad (3.10)$$

where μ and λ are the Lamé parameters, $\operatorname{tr}(\boldsymbol{\varepsilon}(\mathbf{u}))$ is the trace of the strain tensor, and I is the identity matrix. The vector n denotes the unit outward normal to the boundary $\partial\Omega$, and the traction on the boundary is given by $A\boldsymbol{\varepsilon}(\mathbf{u})n$. The boundary $\partial\Omega$ is partitioned into four mutually disjoint parts: the clamped boundary Γ_D , the Neumann boundary Γ_N , the free boundary Γ , and the potential contact boundary Γ_C . On Γ_D , the displacement is fixed to zero, corresponding to fully clamped support. On

the free boundary Γ , no external traction is applied, so we impose the homogeneous Neumann condition $A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n} = 0$. On the Neumann boundary Γ_N , a prescribed traction P is applied: $A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n} = P$. The most critical component of the boundary is Γ_C , where unilateral contact with a rigid, non-deformable obstacle may occur.

To analyze this problem rigorously, we adopt a variational inequality formulation. Let

$$H_{\Gamma_D}^1(\Omega)^2 = \{\mathbf{v} \in H^1(\Omega)^2 \mid \mathbf{v} = 0 \text{ on } \Gamma_D\} \quad (3.11)$$

be the Sobolev space of vector-valued functions that vanish on the clamped part of the boundary. The admissible set of displacements is then defined as:

$$K(\Omega) = \{\mathbf{v} \in H_{\Gamma_D}^1(\Omega)^2 \mid \mathbf{v} = 0 \text{ on } \Gamma_D, \text{ and } \mathbf{v} \cdot \mathbf{n} \leq 0 \text{ a.e. on } \Gamma_C\}. \quad (3.12)$$

The variational inequality associated with the Signorini problem then seeks $\mathbf{u} \in K(\Omega)$ such that:

$$\int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{u}) \, dx \geq \int_{\Omega} \mathbf{f} \cdot (\mathbf{v} - \mathbf{u}) \, dx \quad \forall \mathbf{v} \in K(\Omega). \quad (3.13)$$

This inequality expresses the mechanical equilibrium of the elastic body subject to the unilateral contact constraints. It implies that the solution u is a minimizer of the total potential energy of the system over the admissible set $K(\Omega)$.

The associated total potential energy functional is given by:

$$E(\Omega, \mathbf{u}) = \frac{1}{2} \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \, dx - \int_{\Omega} \mathbf{f} \cdot \mathbf{u} \, dx - \int_{\Gamma_N} P \cdot \mathbf{u} \, ds. \quad (3.14)$$

In the absence of body forces (i.e., when $\mathbf{f} = 0$), this reduces to the pure elastic energy stored in the material:

$$E(\Omega, \mathbf{u}) = \frac{1}{2} \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \, dx - \int_{\Gamma_N} P \cdot \mathbf{u} \, ds. \quad (3.15)$$

To investigate the influence of structural geometry on mechanical performance, while simultaneously achieving material efficiency and geometric regularity, we formulate the structural design problem as a minimization task. The objective functional is defined as follows:

$$\min_{\Omega \in \mathcal{O}_k} J(\Omega) := E(\Omega, \mathbf{u}) + \lambda|\Omega| + \mu (\max(0, \ell(\partial\Omega) - c))^2. \quad (3.16)$$

Here, Ω represents the geometric domain occupied by the structure, and $\mathbf{u}$ denotes the elastic displacement field within Ω , which satisfies the governing linear elasticity equations along with the appropriate contact boundary conditions. The term $E(\Omega, \mathbf{u})$

is the elastic potential energy, reflecting the deformation energy under external loads. The symbol $|\Omega|$ denotes the area of the structure (i.e., volume in two dimensions), and $\ell(\partial\Omega)$ is the total length of the boundary, also referred to as the perimeter. The constants $\lambda > 0$ and $\mu > 0$ serve as weighting parameters for penalizing area and perimeter, respectively, while the positive constant $c > 0$ sets a threshold for allowable boundary length.

The first term in the objective functional, $E(\Omega, \mathbf{u})$, aims to minimize the internal elastic energy of the structure under external loading, thereby achieving a design with high mechanical efficiency. However, if this energy term is considered in isolation, the optimal solution may tend toward an unbounded expansion of the structure in order to distribute stress more evenly and reduce deformation, artificially lowering the energy. To avoid such unrealistic behavior, we introduce the area penalty term $\lambda|\Omega|$ to constrain the overall size of the structure, thus incorporating material usage into the optimization objective. This is especially relevant in lightweight design, where minimizing material consumption is critical while maintaining structural integrity.

On the other hand, to suppress the appearance of highly irregular or oscillatory boundaries in the optimal shape, we include a perimeter penalty term $\mu(\max(0, \ell(\partial\Omega) - c))^2$ in the functional. This term remains inactive when the perimeter is below the threshold c , but increases rapidly when the boundary length exceeds it, effectively discouraging geometric over-complexity. Such a design is not only advantageous for manufacturability but also enhances the structural stability and durability. The perimeter constraint thus acts as a regularization mechanism commonly used in geometric control and shape optimization.

3.2.1 Shape sensitivity

The shape differentiability of shape functional in (3.16) follows by the marginal function differentiability in Mathematical Programming. Under our assumptions "the derivative of minimum is given by the minimum of derivative". It is known that we have only the conical differentiability of the solution to variational inequality with respect to the shape (Sokolowski and Zolesio, 1992), thus the shape derivative $\mathbf{u}'$ does exist in a weak sense as a directional derivative (Sokolowski and Zolesio, 1992). Nevermind, we present in this section the evaluation of the shape gradient for the functional in (3.16) which coincide with the shape gradient in the case of classical differentiability. The classical differentiability occurs under the strict complementarity assumption only, however the result obtained in this section is valid in general case.

To analyze the behavior of the solution to the Signorini problem under small perturbations of the domain, we introduce a class of admissible shape variations. Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with boundary $\partial\Omega$ decomposed into disjoint, sufficiently smooth components: Γ_D , Γ_N , Γ_C , and Γ . We consider shape perturbations generated by a smooth vector field $V \in C^1(\mathbb{R}^2; \mathbb{R}^2)$, which induces a family of diffeomorphisms $F_t : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ defined by

$$F_t(x) := x + tV(x), \quad t \in \mathbb{R}, \quad |t| \ll 1. \quad (3.17)$$

For sufficiently small t , the mapping F_t is a C^1 -diffeomorphism onto its image. The perturbed domain is then defined as

$$\Omega_t := F_t(\Omega), \quad (3.18)$$

and the corresponding perturbed boundary components are given by $\Gamma_{D,t} := F_t(\Gamma_D)$, $\Gamma_{N,t} := F_t(\Gamma_N)$, $\Gamma_{S,t} := F_t(\Gamma_C)$, and $\Gamma_t := F_t(\Gamma)$, preserving the original boundary decomposition under the deformation. The unit outward normal vector field on $\partial\Omega_t$ is denoted by n^t , and it varies smoothly with t due to the regularity of F_t .

This framework allows us to systematically investigate how the solution $\mathbf{u}^t$ of the Signorini problem on Ω_t behaves as $t \rightarrow 0$, i.e., as the domain smoothly returns to its original configuration Ω . In the following lemma, we show that the solution $\mathbf{u}^t$, when pulled back to the reference domain Ω , converges strongly to the unperturbed solution $\mathbf{u}$ in the H^1 -norm.

Lemma 3.2.1. *Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with sufficiently smooth boundary, and let $V \in C^1(\mathbb{R}^2; \mathbb{R}^2)$ denote a fixed smooth vector field. For each $t > 0$, define the perturbed domain by $\Omega_t := F_t(\Omega)$, where $F_t(x) := x + tV(x)$ is a diffeomorphism for small enough t . Let $\mathbf{u}^t$ be the solution to the Signorini problem on Ω_t , and let $\mathbf{u}$ be the solution on the original domain Ω . Define the pullback $\mathbf{u}_t := \mathbf{u}^t \circ F_t$. Then as $t \rightarrow 0$, we have the strong convergence $\mathbf{u}_t \rightarrow \mathbf{u}$ in $H^1(\Omega)^2$.*

Proof. On the perturbed domain Ω_t , the solution $\mathbf{u}^t$ satisfies the analogous variational inequality with modified bilinear form and right-hand side, and admissible set K_t . Pulling back $\mathbf{u}^t$ via F_t , we define $\mathbf{u}_t := \mathbf{u}^t \circ F_t$, and transform the variational inequality to the fixed domain Ω .

Using standard transformation rules under diffeomorphisms, the pullback of the bilinear form takes the form

$$a_t(\mathbf{u}_t, \mathbf{v}) = \int_{\Omega} A_t(x) \boldsymbol{\varepsilon}(\mathbf{u}_t) : \boldsymbol{\varepsilon}(\mathbf{v}) J_t(x) dx, \quad (3.19)$$

where $A_t(x) := A(F_t(x))$ and $J_t(x)$ is the Jacobian determinant $\det DF_t(x)$. Similarly, the right-hand side becomes

$$\ell_t(\mathbf{v}) = \int_{\Omega} f(F_t(x)) \cdot \mathbf{v}(x) J_t(x) dx + \int_{\Gamma_N} P(F_t(x)) \cdot \mathbf{v}(x) j_t(x) ds, \quad (3.20)$$

with j_t the surface Jacobian.

Since $F_t \rightarrow \text{Id}$ in C^1 , it follows that $A_t \rightarrow A$, $J_t \rightarrow 1$, and the data $f(F_t)$, $P(F_t)$ converge strongly to f , P , respectively.

Hence, $a_t(\mathbf{u}, \mathbf{v}) \rightarrow a(\mathbf{u}, \mathbf{v})$ and $\ell_t(\mathbf{v}) \rightarrow \ell(\mathbf{v})$ for all smooth test functions.

Furthermore, the admissible sets K_t pulled back to Ω converge to K in the sense of Mosco, due to the smoothness of F_t and the continuity of the unilateral constraint. Therefore, the family of variational inequalities on Ω corresponding to the pulled-back problems satisfies the convergence framework for variational inequalities, and the solutions $\mathbf{u}_t$ converge weakly in $H^1(\Omega)^2$ to $\mathbf{u}$.

Finally, uniform coercivity of the bilinear forms a_t and the convergence of the data ensure that this convergence is in fact strong. Thus, we conclude that $\|\mathbf{u}_t - \mathbf{u}\|_{H^1(\Omega)} \rightarrow 0$ as $t \rightarrow 0$, which completes the proof. $\square$

Lemma 3.2.2. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain, and let $F_t(x) = x + tV(x)$, with $V \in C_c^1(\mathbb{R}^d; \mathbb{R}^d)$, define a perturbation of the domain. Let $\Omega_t = F_t(\Omega)$ be the perturbed domain. Let $G : \mathbb{R}^d \rightarrow \mathbb{R}$ be a fixed integrable function. Then the Eulerian (shape) derivative of the integral over Ω_t is given by:*

$$\left. \frac{d}{dt} \int_{\Omega_t} G(x) dx \right|_{t=0} = \int_{\Omega} G(x) \operatorname{div} V(x) dx, \quad (3.21)$$

or, equivalently,

$$\left. \frac{d}{dt} \int_{\Omega_t} G(x) dx \right|_{t=0} = \int_{\partial\Omega} G(x) V(x) \cdot n(x) ds, \quad (3.22)$$

provided G is sufficiently regular (e.g., continuous) near $\partial\Omega$.

Moreover, if the integrand also depends on t , e.g., $G(x, t) = G(x) \cdot \phi^t(x)$, where ϕ^t is a t -dependent state variable (such as a PDE solution), and $\dot{\phi}(x) := \left. \frac{d}{dt} \phi^t(x) \right|_{t=0}$ denotes its material derivative, then

$$\left. \frac{d}{dt} \int_{\Omega_t} G(x) \cdot \phi^t(x) dx \right|_{t=0} = \int_{\Omega} G(x) \cdot \dot{\phi}(x) dx + \int_{\Omega} G(x) \cdot \phi(x) \operatorname{div} V(x) dx. \quad (3.23)$$

In linearized elasticity, the strain tensor associated with the displacement field $\mathbf{u}_t : \Omega_t \rightarrow \mathbb{R}^d$ is defined as

$$\boldsymbol{\varepsilon}(\mathbf{u}_t) = \frac{1}{2} (\nabla \mathbf{u}_t + (\nabla \mathbf{u}_t)^T). \quad (3.24)$$

We define the pullback displacement $\mathbf{u}^t(x) := \mathbf{u}_t(F_t(x))$. The gradient of $\mathbf{u}_t$ can be related to $\mathbf{u}^t$ via:

$$\nabla \mathbf{u}_t(x) = \nabla \mathbf{u}^t(F_t^{-1}(x)) \cdot DF_t^{-1}(x), \quad (3.25)$$

and since $DF_t(x) = I + t\nabla V(x)$, we can express the strain tensor in the reference domain as:

$$\boldsymbol{\varepsilon}^t(\mathbf{u}^t)(x) := \frac{1}{2} \left(\nabla \mathbf{u}^t(x) \cdot DF_t(x)^{-1} + DF_t(x)^{-T} \cdot (\nabla \mathbf{u}^t(x))^T \right). \quad (3.26)$$

Taking the derivative at $t = 0$, we obtain the material derivative of the strain tensor:

$$\left. \frac{d}{dt} \boldsymbol{\varepsilon}^t(\mathbf{u}^t)(x) \right|_{t=0} = \boldsymbol{\varepsilon}(\dot{\mathbf{u}})(x) - (\nabla \mathbf{u}(x) \nabla V(x))^{\text{sym}}, \quad (3.27)$$

where $(\cdot)^{\text{sym}}$ denotes the symmetric part of a matrix:

$$(\nabla \mathbf{u} \nabla V)^{\text{sym}} := \frac{1}{2} \left(\nabla \mathbf{u} \nabla V + (\nabla \mathbf{u} \nabla V)^T \right). \quad (3.28)$$

Moreover, the shape derivative $\mathbf{u}'$ is related to the material derivative $\dot{\mathbf{u}}$ via the transport relation:

$$\mathbf{u}' = \dot{\mathbf{u}} - \nabla \mathbf{u} \cdot V, \quad (3.29)$$

which leads to the following shape derivative of the strain tensor:

$$\boldsymbol{\varepsilon}'(u) = \boldsymbol{\varepsilon}(\dot{\mathbf{u}} - \nabla \mathbf{u} \cdot V) = \boldsymbol{\varepsilon}(\dot{\mathbf{u}}) - (\nabla \mathbf{u} \nabla V)^{\text{sym}}. \quad (3.30)$$

Let $\mathbf{u}^t(x) := \mathbf{u}_t(F_t(x))$ denote the pullback of the displacement field, and let $J_t(x) := \det(DF_t(x))$ and $j_t(x) := \|DF_t^{-T}(x)n(x)\|$ denote the volume and surface Jacobians, respectively. Then we rewrite the energy as:

$$E(\Omega_t, \mathbf{u}_t) = \frac{1}{2} \int_{\Omega} A \boldsymbol{\varepsilon}^t(\mathbf{u}^t) : \boldsymbol{\varepsilon}^t(\mathbf{u}^t) J_t dx - \int_{\Omega} f^t \cdot \mathbf{u}^t J_t dx - \int_{\Gamma_N} P^t \cdot \mathbf{u}^t j_t ds, \quad (3.31)$$

where $\boldsymbol{\varepsilon}^t(\mathbf{u}^t)$ is the transformed strain tensor under the deformation, and $f^t = f \circ F_t$, $P^t = P \circ F_t$ are the pullbacks of the data.

Differentiating the energy functional

$$E(\Omega_t, \mathbf{u}_t) = \frac{1}{2} \int_{\Omega_t} A \boldsymbol{\varepsilon}(\mathbf{u}_t) : \boldsymbol{\varepsilon}(\mathbf{u}_t) dx - \int_{\Omega_t} f \cdot \mathbf{u}_t dx - \int_{\Gamma_{N,t}} P \cdot \mathbf{u}_t ds \quad (3.32)$$

with respect to the domain deformation induced by the smooth velocity field $V \in C_c^1(\mathbb{R}^d; \mathbb{R}^d)$, we apply standard tools from shape calculus. Specifically, we perform a pullback of all quantities defined on the moving domain Ω_t to the reference domain Ω

via the transformation $F_t(x) = x + tV(x)$, and use the chain rule to compute the total derivative at $t = 0$.

Differentiating this expression (3.31) at $t = 0$, we make use of the following key identities:

The derivative of the volume element:

$$\left. \frac{d}{dt} J_t \right|_{t=0} = \operatorname{div} V, \quad (3.33)$$

The derivative of the surface element on Γ_N :

$$\left. \frac{d}{dt} j_t \right|_{t=0} = \operatorname{div}_\Gamma V, \quad (3.34)$$

The derivative of the strain tensor:

$$\left. \frac{d}{dt} \boldsymbol{\varepsilon}^t(\mathbf{u}^t) \right|_{t=0} = \boldsymbol{\varepsilon}(\dot{\mathbf{u}}) - (\nabla \mathbf{u} \nabla V)^{\operatorname{sym}}, \quad (3.35)$$

where $\dot{\mathbf{u}} := \left. \frac{d}{dt} \mathbf{u}^t \right|_{t=0}$ is the material derivative of $\mathbf{u}_t$, and $(\cdot)^{\operatorname{sym}}$ denotes the symmetric part of a tensor. Additionally, the shape derivative $\mathbf{u}'$ is related to the material derivative by

$$\mathbf{u}' = \dot{\mathbf{u}} - \nabla \mathbf{u} \cdot V. \quad (3.36)$$

Substituting all these into the expression for $E(\Omega_t, \mathbf{u}_t)$, and differentiating term by term, we obtain:

$$\begin{aligned} dE(\Omega)(V) &= \left. \frac{d}{dt} \frac{1}{2} \int_{\Omega} A \boldsymbol{\varepsilon}^t(\mathbf{u}^t) : \boldsymbol{\varepsilon}^t(\mathbf{u}^t) J_t dx \right|_{t=0} - \left. \frac{d}{dt} \int_{\Omega} f^t \cdot \mathbf{u}^t J_t dx \right|_{t=0} \\ &\quad - \left. \frac{d}{dt} \int_{\Gamma_N} P^t \cdot \mathbf{u}^t j_t ds \right|_{t=0}. \end{aligned} \quad (3.37)$$

Computing each term individually, we have:

$$\left. \frac{d}{dt} \int_{\Omega} A \boldsymbol{\varepsilon}^t(\mathbf{u}^t) : \boldsymbol{\varepsilon}^t(\mathbf{u}^t) J_t dx \right|_{t=0} = \int_{\Omega} A \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}') dx + \int_{\Omega} \frac{1}{2} A \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \operatorname{div} V dx \quad (3.38)$$

and

$$\left. \frac{d}{dt} \int_{\Omega} f^t \cdot \mathbf{u}^t J_t dx \right|_{t=0} = \int_{\Omega} f \cdot \mathbf{u} \operatorname{div} V dx + \int_{\Omega} f \cdot \dot{\mathbf{u}} dx = \int_{\Omega} f \cdot \mathbf{u} \operatorname{div} V dx + \int_{\Omega} f \cdot (\mathbf{u}' + \nabla \mathbf{u} \cdot V) dx. \quad (3.39)$$

and

$$\left. \frac{d}{dt} \int_{\Gamma_N} P^t \cdot \mathbf{u}^t j_t ds \right|_{t=0} = \int_{\Gamma_N} P \cdot \mathbf{u} \operatorname{div}_\Gamma V ds + \int_{\Gamma_N} P \cdot \mathbf{u}' ds. \quad (3.40)$$

Combining all of these, and rearranging, we arrive at the complete expression for the Eulerian derivative:

$$\begin{aligned}
dE(\Omega)(V) &= \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}') \, dx + \int_{\Omega} \frac{1}{2} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \operatorname{div} V \, dx \\
&\quad - \int_{\Omega} f \cdot \mathbf{u} \operatorname{div} V \, dx - \int_{\Omega} f \cdot \mathbf{u}' \, dx \\
&\quad - \int_{\Gamma_N} P \cdot \mathbf{u} \operatorname{div}_{\Gamma} V \, ds - \int_{\Gamma_N} P \cdot \mathbf{u}' \, ds.
\end{aligned} \tag{3.41}$$

This expression represents the total derivative of the energy with respect to the domain deformation.

To eliminate the terms involving $\mathbf{u}'$, we exploit the fact that $\mathbf{u}'$ satisfies a variational inequality characterizing the material derivative of a solution to a Signorini problem. More precisely, $\mathbf{u}'$ is the unique solution to

$$\int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}') : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{u}') \, dx \geq \int_{\Omega} \mathcal{R}(\mathbf{u}, V) \cdot (\mathbf{v} - \mathbf{u}') \, dx + \int_{\Gamma_N} \mathcal{R}_{\Gamma}(\mathbf{u}, V) \cdot (\mathbf{v} - \mathbf{u}') \, ds, \quad \forall \mathbf{v} \in T_{\mathbf{u}}(K), \tag{3.42}$$

where the residual terms due to shape variation are given by Sokolowski and Zolesio, 1992

$$\mathcal{R}(\mathbf{u}, V) = \left(\frac{1}{2} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) - f \cdot \mathbf{u} \right) \operatorname{div} V - A\boldsymbol{\varepsilon}(\mathbf{u}) : (\nabla \mathbf{u} \nabla V)^{\operatorname{sym}} - f, \tag{3.43}$$

$$\mathcal{R}_{\Gamma}(\mathbf{u}, V) = -P \operatorname{div}_{\Gamma} V.$$

By testing the variational inequality with $v = 0$, we obtain an upper bound on the $\mathbf{u}'$ -dependent terms. Substituting this bound into the shape derivative expression yields the following inequality:

$$\begin{aligned}
\int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}') : \boldsymbol{\varepsilon}(\mathbf{u}') \, dx + \int_{\Omega} f \cdot \mathbf{u}' \, dx + \int_{\Gamma_N} P \cdot \mathbf{u}' \, ds &\leq \int_{\Omega} \left(\frac{1}{2} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) - f \cdot \mathbf{u} \right) \operatorname{div} V \, dx \\
&\quad - \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : (\nabla \mathbf{u} \nabla V)^{\operatorname{sym}} \, dx - \int_{\Gamma_N} P \cdot \mathbf{u} \operatorname{div}_{\Gamma} V \, ds.
\end{aligned} \tag{3.44}$$

Substituting this into the expression for $dE(\Omega)(V)$, the terms involving $\mathbf{u}'$ cancel, and we obtain the simplified Eulerian derivative:

$$\begin{aligned}
dE(\Omega)(V) &= \int_{\Omega} \left(\frac{1}{2} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) - f \cdot \mathbf{u} \right) \operatorname{div} V \, dx - \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : (\nabla \mathbf{u} \nabla V)^{\operatorname{sym}} \, dx \\
&\quad - \int_{\Gamma_N} P \cdot \mathbf{u} \operatorname{div}_{\Gamma} V \, ds.
\end{aligned} \tag{3.45}$$

Furthermore, under sufficient regularity of u and V , and assuming that V extends smoothly to the boundary, and $V = 0$ on $\Gamma_D \cup \Gamma_N$, we may invoke the divergence theorem to express the Eulerian derivative in Hadamard form:

$$dE(\Omega)(V) = \int_{\Gamma} \left(\frac{1}{2} A \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) - f \cdot \mathbf{u} \right) (V \cdot \mathbf{n}) ds \quad (3.46)$$

where $\mathbf{n}$ denotes the outward unit normal to $\partial\Omega$. This Hadamard structure reveals that the shape derivative depends only on the normal component of the velocity field at the boundary, weighted by the local mechanical energy density, and is thus essential for the derivation of shape gradients in optimization problems.

3.2.2 Phase field method

To enhance the numerical stability and convergence of gradient flow equations, we adopt a phase field approach based on a second-order regularization of the energy functional. This method fundamentally replaces the traditional binary, discontinuous geometric representation of the design domain with a continuous phase field variable, enabling a variationally well-posed and differentiable framework for shape optimization.

Specifically, we consider a bounded computational domain $D \subset \mathbb{R}^d$, which contains an unknown subdomain $\Omega \Subset D$ representing the target inclusion. The objective is to determine the optimal shape of Ω that minimizes a given energy functional depending on both the geometry and a physical state variable. In classical shape optimization Harald Garcke and Lam, 2018; Hu et al., 2023; Qian et al., 2022; Tan et al., 2025, the geometry of Ω is often described using the characteristic function χ_1 , which takes the value 1 inside Ω and 0 outside. The associated binary design variable

$$\rho = 2\chi_1 - 1$$

then takes values in $\{-1, 1\}$, representing material and void regions, respectively.

However, this discrete representation is non-differentiable and unsuitable for gradient-based numerical optimization. The phase field method overcomes this difficulty by introducing a continuous function $\varphi : D \rightarrow \mathbb{R}$, known as the phase field or order parameter. Under this formulation, the material domain Ω is approximated by the set $\{\varphi > 0\}$, and the surrounding void region by $\{\varphi < 0\}$. The interface between materials is diffused and approximated by the level set $\{\varphi = 0\}$, forming a narrow transition layer referred to as the diffuse interface. The phase field φ smoothly transitions between values near $+1$ and -1 , effectively capturing geometric information in a regularized fashion.

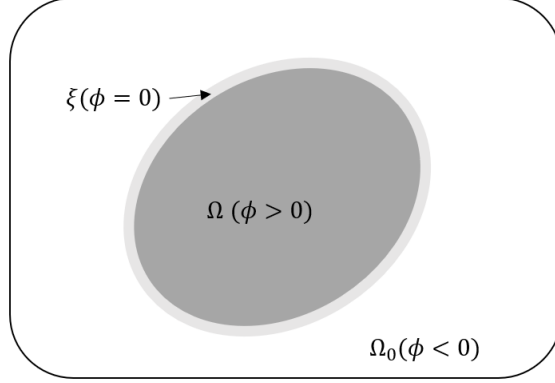


Figure 3.2: The domain $D = \Omega \cup \Omega_0 \cup \xi$ represented by the phase field function

To model the energetic contribution of this transition, we introduce the classical double-well potential:

$$W(\varphi) = \frac{1}{2}(\varphi^2 - 1)^2, \quad (3.47)$$

which has minima at $\varphi = \pm 1$ and penalizes intermediate values. This potential promotes phase separation and enforces stability of the pure phases. Based on this potential, we define the regularized phase field functional $\mathcal{G}_\epsilon$ as:

$$\mathcal{G}_\epsilon(\varphi) = \frac{1}{2} \int_D \frac{1}{\epsilon} \left(-\epsilon \Delta \varphi + \frac{1}{\epsilon} W'(\varphi) \right)^2 dx + \frac{\gamma}{2} \int_D \left(\frac{\epsilon}{2} |\nabla \varphi|^2 + \frac{1}{\epsilon} W(\varphi) \right) dx, \quad (3.48)$$

where $\epsilon > 0$ controls the width of the diffuse interface and $\gamma > 0$ is a regularization parameter. The first term arises from the squared chemical potential, and is typically associated with Cahn-Hilliard-type gradient flows. It imposes higher regularity and stabilizes the evolution of diffuse interfaces in time-dependent phase field models. Since the first term involves a second-order differential operator, $\mathcal{G}_\epsilon$ is only finite on functions $\varphi \in W^{2,2}(D)$, and we set $\mathcal{G}_\epsilon(\varphi) = +\infty$ otherwise to enforce regularity constraints variationally.

To compute descent directions or construct gradient flow dynamics, we need to evaluate the variational derivative of $\mathcal{G}_\epsilon$ with respect to φ . Given a smooth perturbation $\delta\varphi$, the first variation is defined as:

$$\left. \frac{d}{d\lambda} \mathcal{G}_\epsilon(\varphi + \lambda \delta\varphi) \right|_{\lambda=0} = \int_D d\mathcal{G}_\epsilon(\varphi) \delta\varphi dx, \quad (3.49)$$

where $d\mathcal{G}_\epsilon$ denotes the L^2 -gradient of the energy functional. Through direct computation, we obtain the explicit expression:

$$d\mathcal{G}_\epsilon = -\frac{1}{\epsilon} \Delta \beta_\epsilon + \frac{1}{\epsilon^3} W''(\varphi) \beta_\epsilon + \frac{\gamma}{2\epsilon} \beta_\epsilon, \quad (3.50)$$

with

$$\beta_\epsilon := W'(\varphi) - \epsilon^2 \Delta \varphi, \quad (3.51)$$

known as the chemical potential, representing the energetic tension between the double-well potential and the interfacial curvature. The term $W''(\varphi)$ denotes the second derivative of the potential and reflects the local curvature of the energy landscape.

We assume $\varphi \in W^{2,2}(D)$, and apply homogeneous Neumann boundary conditions

$$\frac{\partial \varphi}{\partial n} = \frac{\partial \beta_\epsilon}{\partial n} = 0 \text{ on } \partial D, \quad (3.52)$$

ensuring the variational form is well-posed.

This phase field formulation provides a powerful and flexible framework for modeling geometry in optimization problems. It enables the treatment of complex topologies without explicitly tracking interfaces, and supports smooth gradient-based algorithms. The second-order regularization promotes stability and robustness in numerical simulations, making the method particularly well-suited for applications in shape optimization, topology design, and multiphase interface evolution.

To derive the first-order variational derivative of the relaxed objective functional $\mathcal{J}^*(\varphi)$ with respect to the phase field variable φ , we consider the following formulation:

$$\mathcal{J}^*(\varphi) = E(\mathbf{u}(\varphi)) + \tilde{\eta} \mathcal{G}_\epsilon(\varphi), \quad (3.53)$$

where $\varphi \in H^1(D)$ is a phase-field function defined over a fixed Lipschitz domain $D \subset \mathbb{R}^d$, and $\tilde{\eta} > 0$ is a regularization parameter. The structural energy $E(\mathbf{u}(\varphi))$ depends implicitly on φ through the displacement field $u = \mathbf{u}(\varphi)$, which solves a Signorini-type variational inequality in the effective material domain $\Omega(\varphi) := \{x \in D \mid \varphi(x) > 0\}$. The regularization term $\mathcal{G}_\epsilon(\varphi)$ penalizes the interfacial energy of $\Omega(\varphi)$ in the sense of a diffuse interface.

Our goal is to compute the directional derivative of $\mathcal{J}^*(\varphi)$ in an arbitrary direction $\delta\varphi \in H^1(D)$, i.e.,

$$\delta \mathcal{J}^*(\varphi)[\delta\varphi] := \left. \frac{d}{d\lambda} \mathcal{J}^*(\varphi + \lambda \delta\varphi) \right|_{\lambda=0}. \quad (3.54)$$

Since $\mathcal{J}^*$ consists of two components, we analyze each term separately before combining them to obtain the full expression for the variational derivative.

The principal analytical challenge lies in differentiating the structural energy $E(\mathbf{u}(\varphi))$, which depends on φ both explicitly—via the material tensor $A(\varphi)$ —and implicitly through the solution $\mathbf{u}(\varphi)$ of the state inequality. The implicit dependence makes direct differentiation of u problematic. However, by employing the sensitivity

analysis of variational inequalities, it is possible to derive an explicit formula for the directional derivative of $E(\mathbf{u}(\varphi))$ without requiring the explicit form of the derivative $\mathbf{u}'$. The result is summarized in the following theorem.

Theorem 3.2.3. *Let $D \subset \mathbb{R}^d$ be a bounded Lipschitz domain, and $\varphi \in H^1(D)$ a phase-field function. Define a material-dependent elasticity tensor:*

$$A(\varphi) = \chi(\varphi)A_1 + (1 - \chi(\varphi))A_0, \quad (3.55)$$

where A_1, A_0 are symmetric, positive definite fourth-order tensors, and $\chi(\varphi)$ is a smooth interpolation function. Let $\mathbf{u}(\varphi)$ be the solution to the Signorini-type variational inequality:

$$\mathbf{u} \in K : \quad \int_D A(\varphi) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{u}) dx \geq \int_D f \cdot (\mathbf{u} - \mathbf{v}) dx \quad \forall \mathbf{v} \in K, \quad (3.56)$$

where $K \subset H^1(D; \mathbb{R}^d)$ is a closed convex set of admissible displacements (e.g., satisfying unilateral boundary constraints). Let

$$E(u) := \frac{1}{2} \int_D A(\varphi) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) dx - \int_D f \cdot \mathbf{u} dx. \quad (3.57)$$

Assume that:

- the mapping $\varphi \mapsto A(\varphi)$ is C^1 ;
- the mapping $\varphi \mapsto \mathbf{u}(\varphi)$ is directionally differentiable in the sense of variational inequalities (cf. Sokolowski and Zolesio, 1992);
- the contact set is regular, and $\mathbf{u}'$, the directional derivative of $\mathbf{u}(\varphi)$, exists in a weak sense and lies in the tangent cone $T_{\mathbf{u}}(K)$ at u .

Then, for any perturbation direction $\delta\varphi \in H^1(D)$, the directional derivative of the energy $E(\mathbf{u}(\varphi))$ satisfies:

$$\delta E(u)[\delta\varphi] := \left. \frac{d}{d\lambda} E(\mathbf{u}(\varphi + \lambda\delta\varphi)) \right|_{\lambda=0} = \frac{1}{2} \int_D \chi'(\varphi)(A_1 - A_0) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \delta\varphi dx. \quad (3.58)$$

Proof. We begin by noting that since $\mathbf{u} = \mathbf{u}(\varphi)$ depends on φ through a variational inequality, the total derivative of $E(\mathbf{u}(\varphi))$ in the direction $\delta\varphi$ is given by:

$$\delta E(\mathbf{u})[\delta\varphi] = \left. \frac{d}{d\lambda} \left[\frac{1}{2} \int_D A(\varphi + \lambda\delta\varphi) \boldsymbol{\varepsilon}(\mathbf{u}^\lambda) : \boldsymbol{\varepsilon}(\mathbf{u}^\lambda) dx - \int_D f \cdot \mathbf{u}^\lambda dx \right] \right|_{\lambda=0}, \quad (3.59)$$

where $\mathbf{u}^\lambda := \mathbf{u}(\varphi + \lambda \delta \varphi)$.

Using the chain rule:

$$\delta E(u)[\delta \varphi] = \frac{1}{2} \int_D \partial_\varphi A(\varphi) \delta \varphi \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) dx + \int_D A(\varphi) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}') dx - \int_D f \cdot \mathbf{u}' dx. \quad (3.60)$$

Recall that $\mathbf{u}'$ satisfies the linearized variational inequality:

$$\mathbf{u}' \in T_{\mathbf{u}}(K) : \int_D A(\varphi) \boldsymbol{\varepsilon}(\mathbf{u}') : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{u}') dx \geq \int_D \mathcal{R}(\mathbf{u}, \delta \varphi) \cdot (\mathbf{v} - \mathbf{u}') dx, \quad \forall \mathbf{v} \in T_{\mathbf{u}}(K), \quad (3.61)$$

where the residual vector is

$$\mathcal{R}(\mathbf{u}, \delta \varphi) = \frac{1}{2} \partial_\varphi A(\varphi) \delta \varphi \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) - \partial_\varphi A(\varphi) \delta \varphi \nabla \mathbf{u}. \quad (3.62)$$

Taking $\mathbf{v} = 0 \in T_{\mathbf{u}}(K)$ as a test function, we obtain:

$$\int_D A(\varphi) \boldsymbol{\varepsilon}(\mathbf{u}') : \boldsymbol{\varepsilon}(\mathbf{u}') dx + \int_D \mathcal{R}(\mathbf{u}, \delta \varphi) \cdot \mathbf{u}' dx \leq 0. \quad (3.63)$$

Thus, inserting back into the original chain rule gives:

$$\delta E(\mathbf{u})[\delta \varphi] \leq \frac{1}{2} \int_D \partial_\varphi A(\varphi) \delta \varphi \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) dx, \quad (3.64)$$

which proves the inequality. Under sufficient regularity assumptions (e.g., if $\mathbf{u}'$ solves the linearized system exactly or if E is differentiable), the inequality becomes an equality:

$$\delta E(\mathbf{u})[\delta \varphi] = \frac{1}{2} \int_D \chi'(\varphi) (A_1 - A_0) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \delta \varphi dx. \quad (3.65)$$

□

The regularization functional $\mathcal{G}_\epsilon(\varphi)$ is given by:

$$\delta \mathcal{G}_\epsilon[\delta \varphi] = \int_D \left[-\frac{1}{\epsilon} \Delta \beta_\epsilon + \left(\frac{1}{\epsilon^3} W''(\varphi) + \frac{\gamma}{2\epsilon} \right) \beta_\epsilon \right] \delta \varphi dx. \quad (3.66)$$

Combining the above two contributions, we obtain the full expression of the first-order variational derivative:

$$\begin{aligned} \delta \mathcal{J}^*(\varphi)[\delta \varphi] &= \delta E(\mathbf{u})[\delta \varphi] + \delta \mathcal{G}_\epsilon[\delta \varphi] \\ &= \frac{1}{2} \int_D \chi'(\varphi) (A_1 - A_0) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) \delta \varphi dx + \tilde{\eta} \int_D \left[-\frac{1}{\epsilon} \Delta \beta_\epsilon + \left(\frac{1}{\epsilon^3} W''(\varphi) + \frac{\gamma}{2\epsilon} \right) \beta_\epsilon \right] \delta \varphi dx. \end{aligned} \quad (3.67)$$

3.2.3 Gradient flow based on Allen-Cahn equation

To enable non-conservative evolution of material distribution during the structural optimization process, we formulate an Allen–Cahn type phase-field gradient flow model within the context of a relaxed phase-field–Signorini variational framework. This model describes the temporal evolution of the phase-field variable $\varphi(x, t)$, which implicitly encodes the geometry of the material region $\Omega(\varphi) := \{x \in D \mid \varphi(x) > 0\}$, by means of an L^2 -gradient descent flow.

We introduce the chemical potential $\mu := \frac{\delta \mathcal{J}^*(\varphi)}{\delta \varphi}$, which serves as the variational derivative of the objective functional in the L^2 -sense. As derived previously, the chemical potential consists of two contributions: one from the structural energy and one from the regularization functional. Specifically, we write:

$$\mu = \frac{1}{2} \chi'(\varphi)(A_1 - A_0) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) + \tilde{\eta} \left(-\frac{1}{\epsilon} \Delta \beta_\epsilon + \left(\frac{1}{\epsilon^3} W''(\varphi) + \frac{\gamma}{2\epsilon} \right) \beta_\epsilon \right), \quad (3.68)$$

where $\chi(\varphi)$ is the material interpolation function, $\beta_\epsilon := W'(\varphi) - \epsilon^2 \Delta \varphi$ is the regularized chemical potential derived from the phase-field energy $\mathcal{G}_\epsilon$.

The Allen–Cahn gradient flow is then defined by:

$$\partial_t \varphi = -\mu, \quad (3.69)$$

which leads to the evolution equation:

$$\partial_t \varphi = -\frac{1}{2} \chi'(\varphi)(A_1 - A_0) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}) + \tilde{\eta} \left(\frac{1}{\epsilon} \Delta \beta_\epsilon - \left(\frac{1}{\epsilon^3} W''(\varphi) + \frac{\gamma}{2\epsilon} \right) \beta_\epsilon \right). \quad (3.70)$$

This partial differential equation governs the time-dependent evolution of the phase field toward local minimizers of the objective functional. The model does not conserve the total phase volume, which is advantageous in topology optimization scenarios where the appearance and disappearance of material are permitted.

The Allen–Cahn model offers several computational advantages: it involves only second-order spatial derivatives, making it numerically more tractable than the fourth-order Cahn–Hilliard model; it naturally supports gradient-based algorithms; and it allows for efficient simulation of complex topological changes without requiring explicit interface tracking. If volume preservation is desired, additional constraints or penalty terms may be incorporated.

Compared to the Cahn–Hilliard model, the Allen–Cahn formulation does not preserve mass but offers a simpler structure and easier implementation. It is particularly

well-suited for shape optimization problems where strict volume conservation is not enforced.

The chemical potential consists of two contributions: the structural energy part and the phase field regularization part. The former is given by

$$\mu^{\text{el}} := \frac{1}{2} \chi'(\varphi) (A_1 - A_0) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u}). \quad (3.71)$$

The regularization part arises from the double-well potential $W(\varphi) = \frac{1}{2}(\varphi^2 - 1)^2$ and its associated second-order term, leading to:

$$\mu^{\text{ph}} := -\frac{1}{\epsilon} \Delta \beta_\epsilon + \left(\frac{1}{\epsilon^3} W''(\varphi) + \frac{\gamma}{2\epsilon} \right) \beta_\epsilon, \quad (3.72)$$

where $\beta_\epsilon := W'(\varphi) - \epsilon^2 \Delta \varphi$ captures the competition between potential energy and interface curvature. The total chemical potential is then expressed as:

$$\mu = \mu^{\text{el}} + \tilde{\eta} \mu^{\text{ph}}. \quad (3.73)$$

To solve the Allen–Cahn evolution equation numerically, we discretize the spatial domain using finite elements and adopt a semi-implicit time-stepping strategy. Let $\mathbf{v}_h \subset H^1(D)$ denote a finite element space, typically consisting of linear or quadratic Lagrange basis functions. The time domain is partitioned uniformly with step size $\Delta t > 0$, and φ^n denotes the discrete solution at time $t^n = n\Delta t$.

At each time step $n \rightarrow n+1$, we follow a two-stage procedure:

Step 1: Solve for the auxiliary variable $\beta_\epsilon^{n+1} \in \mathbf{v}_h$ via the following variational formulation:

$$\int_D \beta_\epsilon^{n+1} \xi \, dx = \int_D (W'(\varphi^n) \xi + \epsilon^2 \nabla \varphi^{n+1} \cdot \nabla \xi) \, dx \quad \forall \xi \in \mathbf{v}_h. \quad (3.74)$$

Here, the nonlinear potential term $W'(\varphi^n)$ is treated explicitly, while the Laplacian term in φ^{n+1} is handled implicitly to improve stability.

Step 2: Update the phase field variable $\varphi^{n+1} \in \mathbf{v}_h$ by solving the discrete Allen–Cahn equation:

$$\int_D \frac{\varphi^{n+1} - \varphi^n}{\Delta t} \eta \, dx + \int_D \mu^{n+1} \eta \, dx = 0 \quad \forall \eta \in \mathbf{v}_h, \quad (3.75)$$

where the total chemical potential is given by

$$\mu^{n+1} = \mu^{\text{el},n} + \tilde{\eta} \mu^{\text{ph},n+1}. \quad (3.76)$$

The elastic part $\mu^{\text{el},n}$ is computed explicitly using the displacement $\mathbf{u}^n$ obtained from the previous time step, while the regularization term $\mu^{\text{ph},n+1}$ is constructed based on the newly updated β_ϵ^{n+1} .

At each time step, the displacement field $\mathbf{u}^n$ must be determined by solving a variational inequality of Signorini type, defined over the material region $\Omega^n = \{x \in D \mid \varphi^n(x) > 0\}$, induced by the current phase field distribution. Specifically:

$$\text{Find } \mathbf{u}^n \in K(\varphi^n), \text{ such that } \int_D A(\varphi^n) \boldsymbol{\varepsilon}(\mathbf{u}^n) : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{u}^n) dx \geq \int_D f \cdot (\mathbf{v} - \mathbf{u}^n) dx, \quad (3.77)$$

with $A(\varphi^n) = \chi(\varphi^n)A_1 + (1 - \chi(\varphi^n))A_0$, and the admissible set $K(\varphi^n)$ encoding the non-penetration boundary condition, $\forall \mathbf{v} \in K(\varphi^n)$. This variational inequality can be solved using penalty methods, Lagrange multipliers, or projection-based iterative solvers.

3.2.4 Topological derivative for Signorini problem

To analyze the sensitivity of the cost functional $\mathcal{J}^*$ with respect to an infinitesimal topological perturbation that is, the removal of a small inclusion at a point $\hat{x} \in D$ by deleting a small ball $B_\epsilon(\hat{x})$ of radius ϵ we introduce the classical notion of the topological derivative, defined as

$$D_T(\hat{x}) := \lim_{\epsilon \rightarrow 0} \frac{\mathcal{J}^*(\Omega_\epsilon) - \mathcal{J}^*(\Omega)}{f(\epsilon)}, \quad (3.78)$$

where $\Omega_\epsilon := \Omega \setminus \overline{B_\epsilon(\hat{x})}$ and $f(\epsilon)$ is a scale factor, typically $f(\epsilon) = \pi\epsilon^2$ in two dimensions. here the topological perturbation is far away from boundary.

Consider the topologically perturbed domain Ω_ϵ and the associated boundary value problem:

$$\left\{ \begin{array}{ll} -\text{div}(A\boldsymbol{\varepsilon}(\mathbf{u}_\epsilon)) = f & \text{in } \Omega_\epsilon, \\ \mathbf{u}_\epsilon = 0 & \text{on } \Gamma_D, \\ A\boldsymbol{\varepsilon}(\mathbf{u}_\epsilon)\mathbf{n} = 0 & \text{on } \Gamma, \\ A\boldsymbol{\varepsilon}(\mathbf{u}_\epsilon)\mathbf{n} = P & \text{on } \Gamma_N, \\ \mathbf{u}_\epsilon \cdot \mathbf{n} \leq 0, \quad (A\boldsymbol{\varepsilon}(\mathbf{u}_\epsilon)\mathbf{n}) \cdot \mathbf{n} \leq 0, \quad (\mathbf{u}_\epsilon \cdot \mathbf{n})((A\boldsymbol{\varepsilon}(\mathbf{u}_\epsilon)\mathbf{n}) \cdot \mathbf{n}) = 0 & \text{on } \Gamma_C. \end{array} \right. \quad (3.79)$$

The solution $\mathbf{u}_\epsilon$ to the boundary value problem (3.79) is understood in the variational sense. For simplicity, we choose $f = 0$. Specifically, $\mathbf{u}_\epsilon$ is the unique minimizer

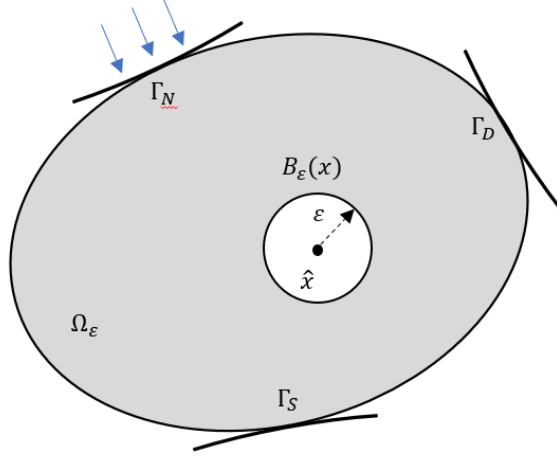


Figure 3.3: Domain with a topological perturbation: $\Omega_\varepsilon = \Omega \setminus \overline{B_\varepsilon}$

of the quadratic energy functional

$$\mathcal{I}_\varepsilon(\varphi) = \frac{1}{2} \int_{\Omega_\varepsilon} A \varepsilon(\varphi) : \varepsilon(\varphi) dx - \int_{\Gamma_N} P \cdot \varphi ds, \quad (3.80)$$

taken over the linear subspace $\mathcal{V}_\varepsilon \subset H^1(\Omega_\varepsilon)$ defined by

$$\mathcal{V}_\varepsilon := \{ \varphi \in H^1(\Omega_\varepsilon) : \varphi = 0 \text{ on } \Gamma_D \}. \quad (3.81)$$

This subspace incorporates the essential (Dirichlet) boundary conditions on Γ_D , while the contact conditions on Γ_C are handled via variational inequalities or convex constraints, depending on the formulation. The functional $\mathcal{I}_\varepsilon$ represents the elastic energy of the system under external loading and boundary interaction in the perturbed domain Ω_ε .

We introduce and define a family of Steklov–Poincaré boundary operators on the outer boundary Γ_R of the region $C(\varepsilon, R)$, which contains a small hole B_ε of radius ε as a localized geometric perturbation.

Let $\Omega_\varepsilon = \Omega \setminus \overline{B_\varepsilon} \subset \mathbb{R}^2$ be a domain containing a small hole B_ε of radius $\varepsilon \rightarrow 0$, centered at a point $\hat{x} \in \Omega$. We assume that $B_\varepsilon \subset B_R$, where B_R is a larger ball. We define the truncated domain as $\Omega_R = \Omega \setminus \overline{B_R}$, which excludes the hole, and define the annular region (or ring) containing the hole as $C(R, \varepsilon) = B_R \setminus \overline{B_\varepsilon}$. In this way, the perturbed domain Ω_ε is naturally decomposed into two subdomains: the outer truncated domain Ω_R and the local neighborhood of the hole $C(R, \varepsilon)$.

The key idea of the approach is to carry out asymptotic analysis on the linear problem within this decomposition, and then to transfer the results to a nonlinear

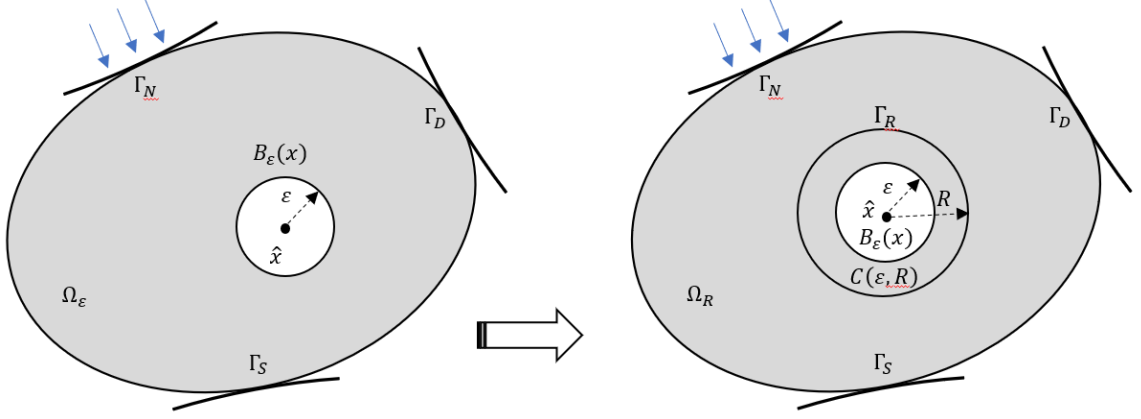


Figure 3.4: The topological perturbation domain is divided into two sub-domain: $\Omega_\varepsilon = \Omega_R \cup C(\varepsilon, R)$

problem posed in the truncated domain Ω_R . This strategy is valid because the unilateral boundary conditions are applied on a contact set $\Gamma_C \subset \Omega_R$, which is assumed to be located far from the hole B_ε and hence well-separated from the ball B_R . This spatial separation allows us to isolate the singular perturbation effects and treat them locally within $C(R, \varepsilon)$, while maintaining regularity in Ω_R for the nonlinear analysis.

We fix a radius $R > 0$ such that the circle (or ball, in the case of $d = 3$) B_R completely contains the hole B_ε . This ensures that the hole lies entirely within a localized subregion, allowing us to define a finite, regular subdomain denoted by Ω_R . This truncated domain serves as a localized approximation of the original domain Ω for the purposes of analysis.

Instead of working directly with the boundary value problem posed on the singularly perturbed domain $\Omega_\varepsilon := \Omega \setminus \overline{B_\varepsilon}$, we introduce an approximation of the problem within the subdomain Ω_R . In this reformulation, the singular geometric perturbation caused by the hole is replaced by a regular perturbation in the form of a nonlocal Steklov–Poincaré boundary operator, which is defined on the artificial interface Γ_R the inner boundary of Ω_R .

This operator captures the influence of the exterior region $\Omega \setminus \Omega_R$ on the interior solution within Ω_R , effectively coupling the two via boundary data. In this way, the geometric perturbation problem is reformulated as a perturbation of boundary conditions, which is more tractable for both analytical and numerical purposes.

Next, we consider the domain decomposition method for problem (3.79), under

the assumption that the contact boundary Γ_C is located away from the topological perturbation (i.e., the small hole), and is included within the subdomain Ω_R , as illustrated in Fig.3.4. In this setting, the Sobolev space $H^1_\Gamma(\Omega_R)^d$ originally defined over Ω_R is replaced by a new convex and closed subset to incorporate the non-negativity constraint on the contact boundary. This subset is defined as:

$$\mathcal{K} := \{ \varphi \in H^1_{\Gamma_D}(\Omega_R) : \varphi \cdot \mathbf{n}|_{\Gamma_C} \geq 0 \}, \quad (3.82)$$

which means we consider all vector-valued functions in $H^1(\Omega_R)^d$ that satisfy the Dirichlet boundary condition on Γ_D , and whose normal component on the contact boundary Γ_C is non-positive almost everywhere. This condition models the non-penetration constraint in the context of unilateral contact, where the displacement in the normal direction cannot be positive on Γ_C .

Given a fixed parameter $\varepsilon > 0$ and a boundary function $v \in H^{1/2}(\Gamma_R)$, the operator $\mathcal{A}_\varepsilon(v)$ is defined via the Neumann trace of the unique solution $\mathbf{w}_\varepsilon$ to the following boundary value problem:

$$\begin{cases} \text{Find } \mathbf{w}_\varepsilon \text{ such that:} \\ -\text{div}(\boldsymbol{\varepsilon}(\mathbf{w}_\varepsilon)) = 0 & \text{in } C(\varepsilon, R), \\ \mathbf{w}_\varepsilon = v & \text{on } \Gamma_R, \\ A\boldsymbol{\varepsilon}(\mathbf{w}_\varepsilon)\mathbf{n} = 0 & \text{on } \partial B_\varepsilon, \end{cases} \quad (3.83)$$

where n denotes the outward unit normal vector on the boundary of $C(\varepsilon, R)$, in particular on Γ_R . Notice that by the definition of operator $\mathcal{A}$, the solution $\mathbf{w}_\varepsilon$ of (3.83) satisfies:

$$\int_{B_R} \boldsymbol{\sigma}(\mathbf{w}_\varepsilon) : \boldsymbol{\varepsilon}(\mathbf{w}_\varepsilon) = \int_{\Gamma_R} \mathcal{A}(\psi) \cdot \psi. \quad (3.84)$$

Setting $\psi = \mathbf{u}|_R$, we have $w = \mathbf{u}|_{B_R}$ and $\mathbf{u}^R = u|_{\Omega_R}$. Thus, we can get $\mathcal{I}(\mathbf{u}) = \mathcal{I}^R(\mathbf{u}^R)$, where the functional $\mathcal{I}^R(\mathbf{u}^R)$ is defined as

$$\mathcal{I}^R(\mathbf{u}^R) := \frac{1}{2} \int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}^R) : \boldsymbol{\varepsilon}(\mathbf{u}^R) - \int_{\Gamma_N} P \cdot \mathbf{u}^R + \frac{1}{2} \int_{\Gamma_R} \mathcal{A}(\mathbf{u}^R) \cdot \mathbf{u}^R, \quad (3.85)$$

with the minimizer $\mathbf{u}^R \in \mathbf{V}_1^R := \mathbf{V}_1(\Omega_R)$ being a solution to the following hemivariational inequality: $\forall \mathbf{v} \in \mathbf{V}_1^R$

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}^R) : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{u}^R) - \int_{\Gamma_N} P \cdot (\mathbf{v} - \mathbf{u}^R) + \int_{\Gamma_R} \mathcal{A}(\mathbf{u}^R) \cdot (\mathbf{v} - \mathbf{u}^R) \geq 0, \quad (3.86)$$

where $\mathbf{V}_1(\Omega_R)$'s definition is similar as $V_1(\Omega)$ except Ω is replaced by Ω_R .

Topological perturbation is characterized by the nucleation of a small circular inclusion $\omega_\zeta(\hat{x}) := B_\zeta$ of radius $0 < \zeta < R$ and center at $\hat{x} \in \Omega$, which is assumed to be far enough from the potential contact region Γ_C . This inclusion is filled with different material properties represented by a piecewise constant function r_ζ defined as

$$r_\zeta = r_\zeta(x) := \begin{cases} 1, & \text{if } x \in \Omega \setminus \overline{B_\zeta}, \\ r, & \text{if } x \in B_\zeta, \end{cases} \quad (3.87)$$

with $r \in \mathbb{R}^+$ being used to represent the contrast of the two material properties.

We consider the perturbed domain in B_R : Given $\psi \in H^{1/2}(\Gamma_R; \mathbb{R}^2)$, find the displacement $\mathbf{w}_\zeta : B_R \mapsto \mathbb{R}^2$, such that

$$\begin{cases} -\operatorname{div}(r_\zeta \boldsymbol{\sigma}(\mathbf{w}_\zeta)) = 0 & \text{in } B_R, \\ \boldsymbol{\sigma}(\mathbf{w}_\zeta) = \mathbb{C} \boldsymbol{\varepsilon}(\mathbf{w}_\zeta) & \text{in } B_R, \\ \mathbf{w}_\zeta = \psi & \text{on } \Gamma_R, \\ \llbracket \mathbf{w}_\zeta \rrbracket = 0 & \text{on } \partial B_\zeta, \\ \llbracket r_\zeta \boldsymbol{\sigma}(\mathbf{w}_\zeta) \rrbracket \mathbf{n} = 0 & \text{on } \partial B_\zeta. \end{cases} \quad (3.88)$$

Then we know the solution $\mathbf{w}_\zeta$ of (3.88) satisfies

$$\int_{B_R} r_\zeta \boldsymbol{\sigma}(\mathbf{w}_\zeta) : \boldsymbol{\varepsilon}(\mathbf{w}_\zeta) = \int_{\Gamma_R} \mathcal{A}_\zeta(\psi) \cdot \psi. \quad (3.89)$$

Setting $\psi = \mathbf{u}_\zeta|_{\Gamma_R}$ we have $\mathbf{w}_\zeta = \mathbf{u}_\zeta|_{B_R}$ and $\mathbf{u}_\zeta^R = \mathbf{u}_\zeta|_{\Omega_R}$, which implies the equality $\mathcal{I}_\zeta(\mathbf{u}_\zeta) = \mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R)$, where the functional $\mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R)$ is written as

$$\mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R) := \frac{1}{2} \int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\zeta^R) : \boldsymbol{\varepsilon}(\mathbf{u}_\zeta^R) - \int_{\Gamma_N} P \cdot \mathbf{u}_\zeta^R + \frac{1}{2} \int_{\Gamma_R} \mathcal{A}_\zeta(\mathbf{u}_\zeta^R) \cdot \mathbf{u}_\zeta^R, \quad (3.90)$$

with the minimizer $\mathbf{u}_\zeta^R \in \mathbf{V}_1^R$ given by the unique solution of the hemivariational inequality:

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\zeta^R) : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{u}_\zeta^R) - \int_{\Gamma_N} P \cdot (\mathbf{v} - \mathbf{u}_\zeta^R) + \int_{\Gamma_R} \mathcal{A}_\zeta(\mathbf{u}_\zeta^R) \cdot (\mathbf{v} - \mathbf{u}_\zeta^R) \geq 0. \quad (3.91)$$

Theorem 3.2.4. *Let $\mathbf{u}^R$ and $\mathbf{u}_\zeta^R$ be solution to (3.86) and (3.91), respectively, and assume that*

$$\mathcal{A}_\zeta = \mathcal{A} - \zeta^2 \mathcal{B} + \mathcal{R}_\zeta, \quad (3.92)$$

in the operator norm $\mathcal{L}(H^{1/2}(\Gamma_R; \mathbb{R}^2); H^{-1/2}(\Gamma_R; \mathbb{R}^2))$, with $\mathcal{B}$ denotes a bounded linear operator and $\|\mathcal{R}_\zeta\|_{\mathcal{L}(H^{1/2}(\Gamma_R; \mathbb{R}^2); H^{-1/2}(\Gamma_R; \mathbb{R}^2))} = o(\zeta^2)$. Then, the following estimate holds:

$$\|\mathbf{u}_\zeta^R - \mathbf{u}^R\|_{H^1(\Omega_R; \mathbb{R}^2)} \leq C_0 \zeta^2. \quad (3.93)$$

Proof. By taking $\mathbf{v} = \mathbf{u}_\zeta^R$ in (3.86) and $\mathbf{v} = \mathbf{u}^R$ in (3.91) and adding them together, we can write

$$\int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\zeta^R - \mathbf{u}^R) : \boldsymbol{\varepsilon}(\mathbf{u}_\zeta^R - \mathbf{u}^R) + \int_{\Gamma_R} [\mathcal{A}_\zeta(\mathbf{u}_\zeta^R) - \mathcal{A}(\mathbf{u}^R)] \cdot (\mathbf{u}_\zeta^R - \mathbf{u}^R) \leq 0. \quad (3.94)$$

Assuming (3.92), we have that

$$\begin{aligned} & \int_{\Omega_R} \boldsymbol{\sigma}(\mathbf{u}_\zeta^R - \mathbf{u}^R) : \boldsymbol{\varepsilon}(\mathbf{u}_\zeta^R - \mathbf{u}^R) + \int_{\Gamma_R} \mathcal{A}(\mathbf{u}_\zeta^R - \mathbf{u}^R) \cdot (\mathbf{u}_\zeta^R - \mathbf{u}^R) \\ & \leq \zeta^2 \int_{\Gamma_R} \mathcal{B}(\mathbf{u}_\zeta^R) \cdot (\mathbf{u}_\zeta^R - \mathbf{u}^R) + o(\zeta^2). \end{aligned} \quad (3.95)$$

and by the coercivity of the bilinear form on the left-hand side of (3.95) it follows

$$C_1 \|\mathbf{u}_\zeta^R - \mathbf{u}^R\|_{H^1(\Omega_R; \mathbb{R}^2)}^2 \leq \zeta^2 \int_{\Gamma_R} \mathcal{B}(\mathbf{u}_\zeta^R) \cdot (\mathbf{u}_\zeta^R - \mathbf{u}^R) + o(\zeta^2). \quad (3.96)$$

We can get by duality and the trace theorem

$$\begin{aligned} \|\mathbf{u}_\zeta^R - \mathbf{u}^R\|_{H^1(\Omega_R; \mathbb{R}^2)}^2 & \leq C_2 \zeta^2 \|\mathcal{B}(\mathbf{u}_\zeta^R)\|_{H^{-1/2}(\Gamma_R; \mathbb{R}^2)} \|\mathbf{u}_\zeta^R - \mathbf{u}^R\|_{H^{1/2}(\Gamma_R; \mathbb{R}^2)} \\ & \leq C_0 \zeta^2 \|\mathbf{u}_\zeta^R - \mathbf{u}^R\|_{H^1(\Omega_R; \mathbb{R}^2)}. \end{aligned} \quad (3.97)$$

We obtain (3.93) with C_0 independent of the small parameter ζ . $\square$

Lemma 3.2.5. *The perturbed energy shape functional $\mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R)$ in (3.90) is differentiable w.r.t. $\zeta \rightarrow 0$. In particular, it admits the asymptotic expansion*

$$\mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R) = \mathcal{I}^R(\mathbf{u}^R) - \frac{\zeta^2}{2} \langle \mathcal{B}(\mathbf{u}^R), \mathbf{u}^R \rangle_{\Gamma_R} + o(\zeta^2). \quad (3.98)$$

Proof. By taking into account that $\mathbf{u}_\zeta^R \in \mathbf{V}_1^R$ is the minimizer of (3.90) and $\mathbf{u}^R \in \mathbf{V}_1^R$ is the minimizer of (3.85), the following inequalities hold true

$$\mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R) - \mathcal{I}^R(\mathbf{u}_\zeta^R) \leq \mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R) - \mathcal{I}^R(\mathbf{u}^R) \leq \mathcal{I}_\zeta^R(\mathbf{u}^R) - \mathcal{I}^R(\mathbf{u}^R). \quad (3.99)$$

Using the definitions of $\mathcal{I}_\zeta^R$ and J^R and considering the expansion (3.92), we have

$$\frac{\mathcal{I}_\zeta^R(\mathbf{u}^R) - \mathcal{I}^R(\mathbf{u}^R)}{\zeta^2} = -\frac{1}{2} \langle \mathcal{B}(\mathbf{u}^R), \mathbf{u}^R \rangle_{\Gamma_R} + \langle \mathcal{R}_\zeta(\mathbf{u}^R), \mathbf{u}^R \rangle_{\Gamma_R}. \quad (3.100)$$

Thus, we can obtain

$$\lim_{\zeta \rightarrow 0^+} \frac{\mathcal{I}_\zeta^R(\mathbf{u}^R) - \mathcal{I}^R(\mathbf{u}^R)}{\zeta^2} = -\frac{1}{2} \langle \mathcal{B}(\mathbf{u}^R), \mathbf{u}^R \rangle_{\Gamma_R}. \quad (3.101)$$

Similarly, we can get the limit on the left of (3.99). Then we conclude that

$$\lim_{\zeta \rightarrow 0^+} \frac{\mathcal{I}_\zeta^R(\mathbf{u}_\zeta^R) - \mathcal{I}^R(\mathbf{u}^R)}{\zeta^2} = -\frac{1}{2} \langle \mathcal{B}(\mathbf{u}^R), \mathbf{u}^R \rangle_{\Gamma_R}. \quad (3.102)$$

□

Lemma 3.2.6. *Novotny and Sokolowski, 2013 The energy inside B_R admits the asymptotic expansion:*

$$\int_{B_R} \boldsymbol{\sigma}_\zeta(\mathbf{w}_\zeta) : \boldsymbol{\varepsilon}(\mathbf{w}_\zeta) = \int_{B_R} \boldsymbol{\sigma}(\mathbf{w}) : \boldsymbol{\varepsilon}(\mathbf{w}) - \zeta^2 \mathbb{P}_r \boldsymbol{\sigma}(\mathbf{w}) : \boldsymbol{\varepsilon}(\mathbf{w}) + o(\zeta^2), \quad (3.103)$$

where the fourth-order isotropic polarization tensor $\mathbb{P}_r$ is given by

$$\mathbb{P}_r = \frac{\pi(1-r)}{1+ra_2} \left((1+a_2) \mathbb{I} + \frac{1}{2} (a_1 - a_2) \frac{1-r}{1+ra_1} \mathbf{I} \otimes \mathbf{I} \right), \quad (3.104)$$

with $0 < r < \infty$ and the parameters a_1, a_2 given by

$$a_1 = \frac{\lambda + \mu}{\mu} \text{ and } a_2 = \frac{\lambda + 3\mu}{\lambda + \mu}. \quad (3.105)$$

By Theorem 3.2.4, we can write

$$\langle \mathcal{A}_\zeta(\phi), \varphi \rangle = \langle \mathcal{A}(\phi), \varphi \rangle - \zeta^2 \langle \mathcal{B}(\phi), \varphi \rangle + o(\zeta^2), \quad \forall \phi, \varphi. \quad (3.106)$$

By Lemma 3.2.6, and (3.106), (3.84), (3.89), it follows that

$$\int_{\Gamma_R} \mathcal{B}(\phi) \cdot \varphi = \mathbb{P}_r \boldsymbol{\sigma}(\phi) : \boldsymbol{\varepsilon}(\varphi), \quad \forall \phi, \varphi. \quad (3.107)$$

Thus, by Lemma 3.2.5 together with Eq. (3.107) we have

$$\mathcal{I}_\zeta(\mathbf{u}_\zeta) - \mathcal{I}(u) = -\frac{1}{2} \zeta^2 \mathbb{P}_r \boldsymbol{\sigma}(u) : \boldsymbol{\varepsilon}(u) + o(\zeta^2). \quad (3.108)$$

By choosing $f(\zeta) = \zeta^2$, the topological derivative of the shape functional is given by

$$\mathcal{T}(\mathbf{x}) = -\frac{1}{2} \mathbb{P}_r \boldsymbol{\sigma}(\mathbf{u}(x)) : \boldsymbol{\varepsilon}(\mathbf{u}(x)), \quad \forall \mathbf{x} \in D \quad (3.109)$$

3.2.5 Topological derivatives combined with phase field method

The explicit form of the topological derivative derived above provides localized sensitivity information, identifying regions where the insertion or removal of infinitesimal

inclusions would most significantly affect the cost functional. While such information is classically used in level set, it can also be seamlessly integrated into a diffuse interface framework. To this end, we incorporate the topological derivative into the phase field evolution equation, thereby enriching the classical Allen–Cahn dynamics with topological sensitivity. This approach allows the optimization process to benefit from both geometric smoothness and topology-adaptive responsiveness within a unified variational framework.

We embed this topological derivative into the phase field evolution via a modified Allen–Cahn equation:

$$\partial_t \varphi = - \left(\frac{\delta \mathcal{J}^*(\varphi)}{\delta \varphi} + \kappa \mathcal{T}(x) \hat{\eta}_\epsilon(\varphi) \right), \quad (3.110)$$

where:

- The first term $\frac{\delta \mathcal{J}^*(\varphi)}{\delta \varphi}$ is the classical phase field variation, accounting for elastic energy and interface regularization;
- The second term introduces the topological modulation via $\mathcal{T}(x)$, multiplied by a smooth window function $\hat{\eta}_\epsilon(\varphi)$ (e.g., interface localization function), ensuring that the topological effect activates only near the diffuse interface;
- $\kappa > 0$ is a tunable parameter controlling the strength of topological influence.

The sign of $\mathcal{T}(x)$ dictates the local energetic favorability of topological changes, and thus guides the evolution of the phase field in the vicinity of the interface:

- When $\mathcal{T}(x) < 0$:

This indicates that introducing a small amount of soft material at point x would decrease the total energy functional, i.e., the topological perturbation is energetically favorable. Since the source term enters the evolution as $-\kappa \mathcal{T}(x)$, we have:

$$-\kappa \mathcal{T}(x) > 0, \quad (3.111)$$

which acts as a positive driving force in the Allen–Cahn equation. This results in:

$$\partial_t \varphi < 0 \quad \Rightarrow \quad \varphi(x, t) \searrow -1, \quad (3.112)$$

meaning that the phase field decreases in value and the material point transitions from a solid state ($\varphi \approx +1$) toward a void or soft material state ($\varphi \approx -1$). This effectively removes material in regions where doing so is energetically beneficial.

- When $\mathcal{T}(x) > 0$:

In this case, inserting soft material at point x would lead to an increase in the total energy, rendering the perturbation unfavorable. Accordingly, the contribution of the topological derivative term becomes:

$$-\kappa\mathcal{T}(x) < 0, \quad (3.113)$$

which introduces a negative driving force, yielding:

$$\partial_t \varphi > 0 \quad \Rightarrow \quad \varphi(x, t) \nearrow +1, \quad (3.114)$$

promoting the retention or growth of solid material in such regions. Thus, the evolution naturally reinforces the current structure wherever it is energetically advantageous to do so.

This mechanism allows the phase field model to autonomously reconstruct material layouts by leveraging the local topological sensitivity encoded in $\mathcal{T}(x)$, guiding the formation or removal of material depending on the sign and magnitude of the topological derivative.

For temporal discretization, a semi-implicit time-stepping scheme is adopted to ensure numerical stability and convergence. Let t^n denote the current time step with time increment Δt , then the discrete update rule reads:

$$\frac{\varphi^{n+1} - \varphi^n}{\Delta t} = - \left(\frac{\delta \mathcal{J}^*(\varphi)}{\delta \varphi} \right) \Big|^{n+1} - \kappa \mathcal{T}^n(x) \hat{\eta}_\epsilon(\varphi^n), \quad (3.115)$$

where higher-order differential terms (such as $-\Delta \varphi$) are treated implicitly, and non-linear terms (such as $W'(\varphi)$, $\chi'(\varphi)$) are evaluated at the previous time step to form a stable semi-implicit approximation.

For spatial discretization, the finite element method is employed. Let $V_h \subset H^1(D)$ be a finite-dimensional function space, e.g., spanned by bilinear or quadratic Lagrange elements. At each time step, the discrete weak formulation reads: find $\varphi_h^{n+1} \in V_h$ such that for all test functions $\mathbf{v}_h \in V_h$,

$$\begin{aligned} & \int_D \frac{\varphi_h^{n+1} - \varphi_h^n}{\Delta t} \mathbf{v}_h \, dx + \int_D \left(\gamma \epsilon \nabla \varphi_h^{n+1} \cdot \nabla \mathbf{v}_h + \frac{\gamma}{\epsilon} W'(\varphi_h^n) \mathbf{v}_h \right) dx \\ &= - \int_D \left(\frac{1}{2} \chi'(\varphi_h^n) (A_1 - A_0) \boldsymbol{\varepsilon}(\mathbf{u}_h^n) : \boldsymbol{\varepsilon}(\mathbf{u}_h^n) + \kappa \mathcal{T}_h^n(x) \hat{\eta}_\epsilon(\varphi_h^n) \right) \mathbf{v}_h \, dx, \end{aligned} \quad (3.116)$$

where $\mathbf{u}_h^n$ is the displacement field corresponding to φ_h^n , obtained by solving the elasticity Signorini variational inequality, and $\mathcal{T}_h^n(x)$ is a finite element approximation of

the topological derivative, typically given by

$$\mathcal{T}_h^n(x) = -\mathbb{P}_r \sigma(\mathbf{u}_h^n(\hat{x})) \cdot \varepsilon(\mathbf{u}_h^n(\hat{x})), \quad (3.117)$$

evaluated at each quadrature point or element centroid and assembled as a load-like term in the update step.

This topology-aware Allen–Cahn evolution scheme achieves unified modeling of geometric evolution and topological restructuring, driven by local sensitivity analysis. The numerical formulation enables efficient and robust material-void interface evolution, without explicit remeshing or hole insertion.

3.2.6 Numerical methods for solving the Signorini problem

When solving the Signorini-type variational inequality in contact mechanics, the inherent nonlinearity and nonsmooth nature of the inequality constraints prevent the direct application of standard linear finite element methods. To address this challenge, we employ the semi-smooth Newton method as a robust and efficient numerical approach for resolving such nonsmooth variational systems.

We consider the following variational inequality: find the displacement field $\mathbf{u} \in K \subset V$ such that

$$a(\mathbf{u}, \mathbf{v} - \mathbf{u}) \geq \ell(\mathbf{u} - \mathbf{v}), \quad \forall \mathbf{v} \in K, \quad (3.118)$$

where $V := H_{\Gamma_D}^1(D)^d$ is the vector-valued Sobolev space with Dirichlet boundary conditions, and K is a closed, convex set representing the unilateral contact constraint (e.g., $\mathbf{u} \cdot \mathbf{n} \leq 0$ on the potential contact boundary Γ_S). The bilinear form $a(\mathbf{u}, \mathbf{v})$ corresponds to the linear elasticity operator, and $\ell(\mathbf{v})$ denotes the external load functional.

To handle the nonsmoothness introduced by the contact constraint, we reformulate the variational inequality as a nonsmooth residual equation:

$$R(\mathbf{u}) = 0, \quad (3.119)$$

where the residual operator R incorporates the contact force via a projection operator.

$$\lambda(\mathbf{u}) = \text{Proj}_{\mathbb{R}^+}(\lambda(\mathbf{u}) - \rho \mathbf{u} \cdot \mathbf{n}), \quad (3.120)$$

Here, the projection operator $\text{Proj}_{\mathbb{R}^+} : \mathbb{R} \rightarrow \mathbb{R}^+$ means projecting a real number onto the set, that is:

$$\text{Proj}_{\mathbb{R}^+}(x) := \begin{cases} x, & \text{if } x \geq 0 \\ 0, & \text{if } x < 0. \end{cases} \quad (3.121)$$

Thus, the total residual $R(\mathbf{u})$ becomes a piecewise differentiable function: smooth in the interior of the feasible region and directionally differentiable at the boundary. This structure allows the use of the semi-smooth Newton method.

Upon finite element discretization, we obtain a nonlinear system $F_h(\mathbf{u}_h) = 0$ in a finite-dimensional space $\mathbf{v}_h$. The semi-smooth Newton iteration proceeds by solving a linearized system at each step:

$$DF_h(\mathbf{u}_h^{(k)}) \delta \mathbf{u}_h^{(k)} = -F_h(\mathbf{u}_h^{(k)}), \quad \mathbf{u}_h^{(k+1)} = \mathbf{u}_h^{(k)} + \alpha_k \delta \mathbf{u}_h^{(k)}, \quad (3.122)$$

where $DF_h(\mathbf{u}_h^{(k)})$ is the generalized Jacobian matrix evaluated at the current iterate $\mathbf{u}_h^{(k)}$, and $\alpha_k \in (0, 1]$ is a damping parameter introduced to ensure global convergence.

The contact boundary Γ_S is discretized into a set of nodes $\mathcal{N}_S$. At each iteration k , we define the active set:

$$\mathcal{A}^{(k)} := \left\{ i \in \mathcal{N}_S \mid (\mathbf{u}_h^{(k)} \cdot \mathbf{n})_i = 0, (\lambda_h^{(k)} \cdot \mathbf{n})_i > 0 \right\}, \quad (3.123)$$

and the inactive set $\mathcal{F}^{(k)} = \mathcal{N}_S \setminus \mathcal{A}^{(k)}$. The Jacobian DF_h is constructed accordingly: contact nodes enforce Dirichlet-like conditions or incorporate penalty terms, while free nodes retain the standard Neumann conditions. Each linearized system in the Newton loop can thus be expressed as a symmetric, possibly semi-definite matrix problem and solved using multigrid or algebraic solvers.

3.2.7 Numerical examples

Example 3.2.1. *In this section, we present a numerical example to illustrate the proposed only phase field method for shape and topology optimization with unilateral contact constraints. We consider a benchmark structure within a fixed rectangular domain $D = [0, 2] \times [0, 2]$. The left boundary is clamped, and a vertical load is applied on a selected portion of the center of the right boundary. The bottom boundary is designated as a contact surface subject to Signorini-type conditions, modeling potential non-penetration against a rigid obstacle.*

The initial material distribution is given by a random smooth phase field function $\varphi_0(x)$, as shown in Figure 3.5b. The optimization proceeds via an Allen–Cahn gradient flow driven by the variational derivative of a regularized energy functional, which includes both structural compliance and interfacial energy terms. The elastic response is solved at each time step through a variational inequality incorporating the contact constraint.

The phase field evolves iteratively, producing increasingly refined material layouts that satisfy the mechanical and geometric constraints. Snapshots of the phase field during the optimization are shown in Figure 3.5, while the final optimized shape is presented in Figure 3.5f. The evolution clearly captures topological transitions such as merging or elimination of features, as well as the active contact zone.

As shown in Figure 3.6, the compliance values eventually level off with increasing iterations, indicating that the optimization process has reached convergence. The final design exhibits a well-defined structural form that is able to effectively transfer loads while respecting contact boundaries.

Figure 3.5a provides a schematic diagram of the problem setup, including boundary conditions and loads, for reference.

Example 3.2.2. This example demonstrates the effectiveness of the proposed phase field method for shape and topology optimization under unilateral contact conditions, using a different configuration of the same benchmark problem introduced previously.

The computational domain is still of L shape $D = ([0, 2] \times [0, 2]) \setminus ([1, 1] \times [1, 1])$, where the upper boundary is fixed (clamped), a vertical force is applied downwards on the central part of the lower right boundary, and the central part of the lower boundary acts as a rigid barrier, enforcing a unilateral non-penetration constraint modeled by a Signorini-type condition, as shown in the figure 3.7a

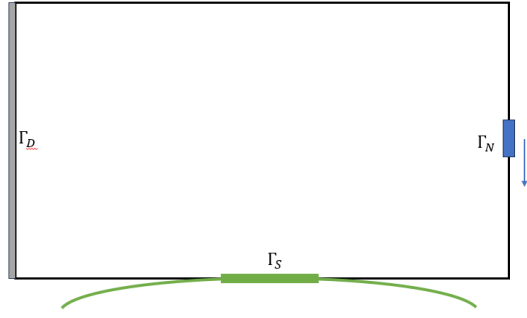
The initial material distribution represented by the phase field function is shown in the figure 3.7b.

The optimization process is driven by the Allen-Cahn gradient flow equation based on the first-order variation of the phase field energy, which combines the minimization of elastic compliance with interface regularization. The displacement field is updated at each time step by solving a variational inequality that captures the contact interaction.

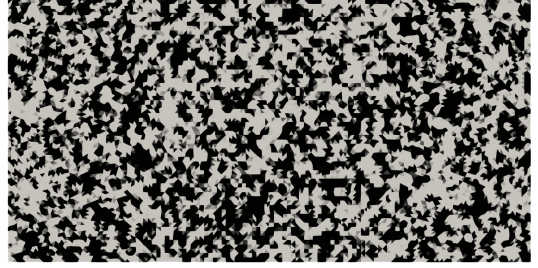
As iterations proceed, the phase field dynamically adjusts to reveal the optimized structural configuration. Figure 3.8 shows the intermediate states in this evolutionary process, highlighting the formation and adjustment of the structural topology under mechanical constraints. The final optimized phase field is shown in Figure 3.8d.

Figure 3.9 plots the change of compliance over time, confirming the effectiveness of the optimization strategy. The results clearly meet the design requirements and successfully take into account the load and contact constraints.

Example 3.2.3. To further demonstrate the effectiveness of the proposed approach, we now consider the same structural setting as in the previous example, but incorporate the



(a) Problem setup



(b) Initial phase field



(c) Iteration 10



(d) Iteration 20



(e) Iteration 50



(f) Iteration 100

Figure 3.5: Shape optimization process for Example 3.2.1. Subfigures (a)–(f) show the model setup, initial phase field and intermediate designs.

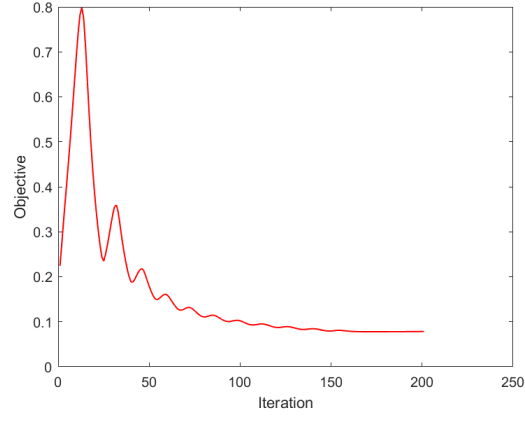


Figure 3.6: Objective function convergence history for Example 3.2.1.

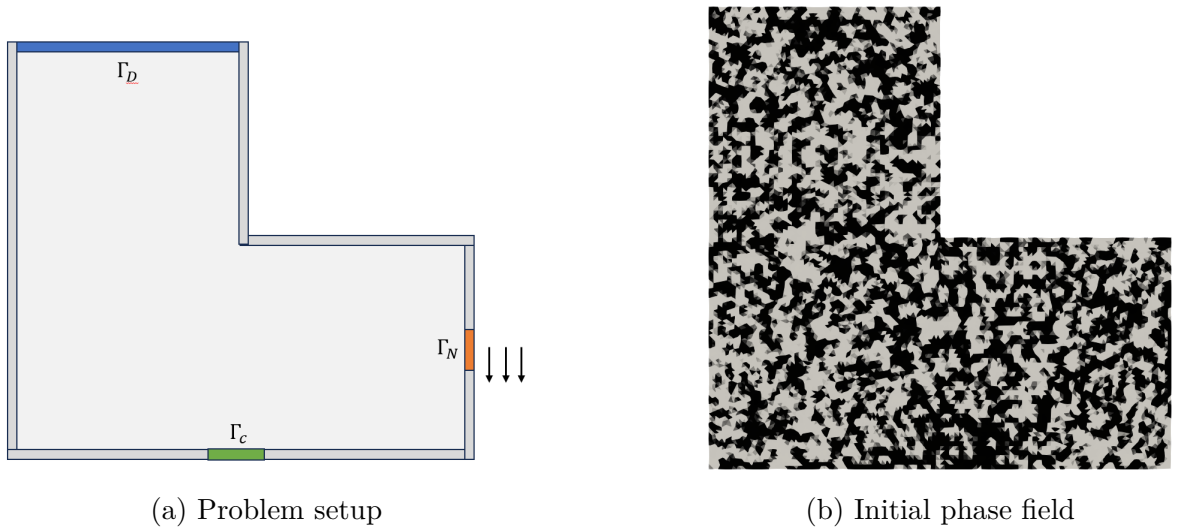


Figure 3.7: the model setup and initial phase field for Example 3.2.2.



(a) Iteration 10



(b) Iteration 50



(c) Iteration 100



(d) Final phase field

Figure 3.8: Shape optimization process for Example 3.2.2. Subfigures show initial phase field and intermediate designs.

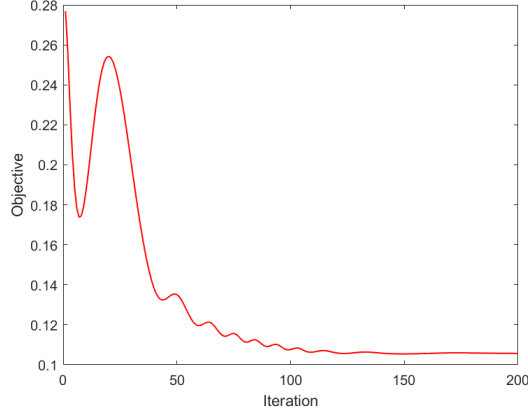


Figure 3.9: Objective function convergence history for Example 3.2.2.

topological derivative into the phase field evolution. This hybrid strategy leverages the smooth interface representation of the phase field method while simultaneously exploiting the localized sensitivity provided by the topological derivative.

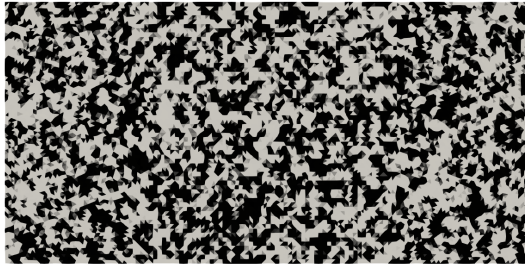
The computational domain, boundary conditions, and external loads remain identical to those described in Figure 3.5a. However, the evolution of the phase field variable $\varphi(x, t)$ is now governed by a modified Allen–Cahn equation augmented with a topological derivative term. This term enables the creation or removal of material in regions where the topological sensitivity $\mathcal{T}(x)$ is significant, thus allowing for more flexible and efficient exploration of the design space.

Figure 3.10 shows the intermediate phase field configurations during the optimization process. Compared to the standard phase field method, the evolution exhibits faster structural emergence and more pronounced topological transitions, including hole nucleation and reconnection. The final optimized layout, shown in Figure 3.10e, displays a complex yet mechanically efficient structure, with contact regions appropriately respected.

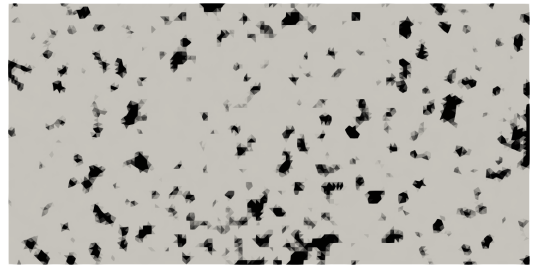
As shown in Figure 3.11, the compliance history shows that the objective function eventually tends to be smooth, that is, converges. In addition, we compared the results with the design obtained using the level set method combined with the same topological derivative formula. As shown in Figure 3.12, this is the optimization graph obtained by combining the level set with the topological derivative. Comparing the two graphs, but because our phase field-based method has natural regularization and differentiability, the initial value can be selected at will, while the results expressed by the classic level set have certain requirements on the selection of the initial region, and our phase field

method combined with the topological derivative method can produce smoother interfaces and better connection structures.

This comparison highlights the advantage of our framework in providing robust numerical performance and high-quality structural designs without requiring reinitialization, interface tracking, or additional topological heuristics.



(a) Initial phase field



(b) Iteration 10



(c) Iteration 20



(d) Iteration 50



(e) Final phase field

Figure 3.10: Shape optimization process for Example 3.2.3. Subfigures show initial phase field and intermediate designs.

Example 3.2.4. In this example, we apply topological derivatives combined with the phase field method to solve the same structural design problem as in example 3.2.2. The domain configuration, boundary conditions, loads, and contact settings remain

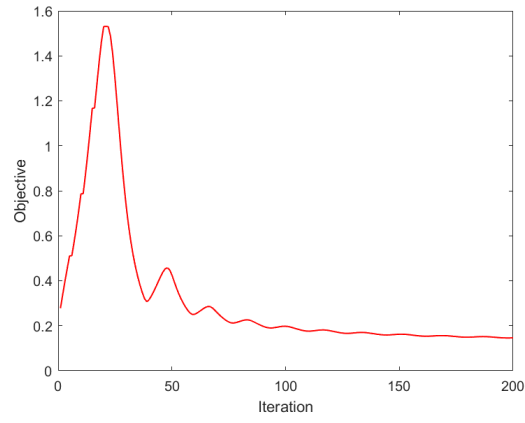


Figure 3.11: Objective function convergence history.

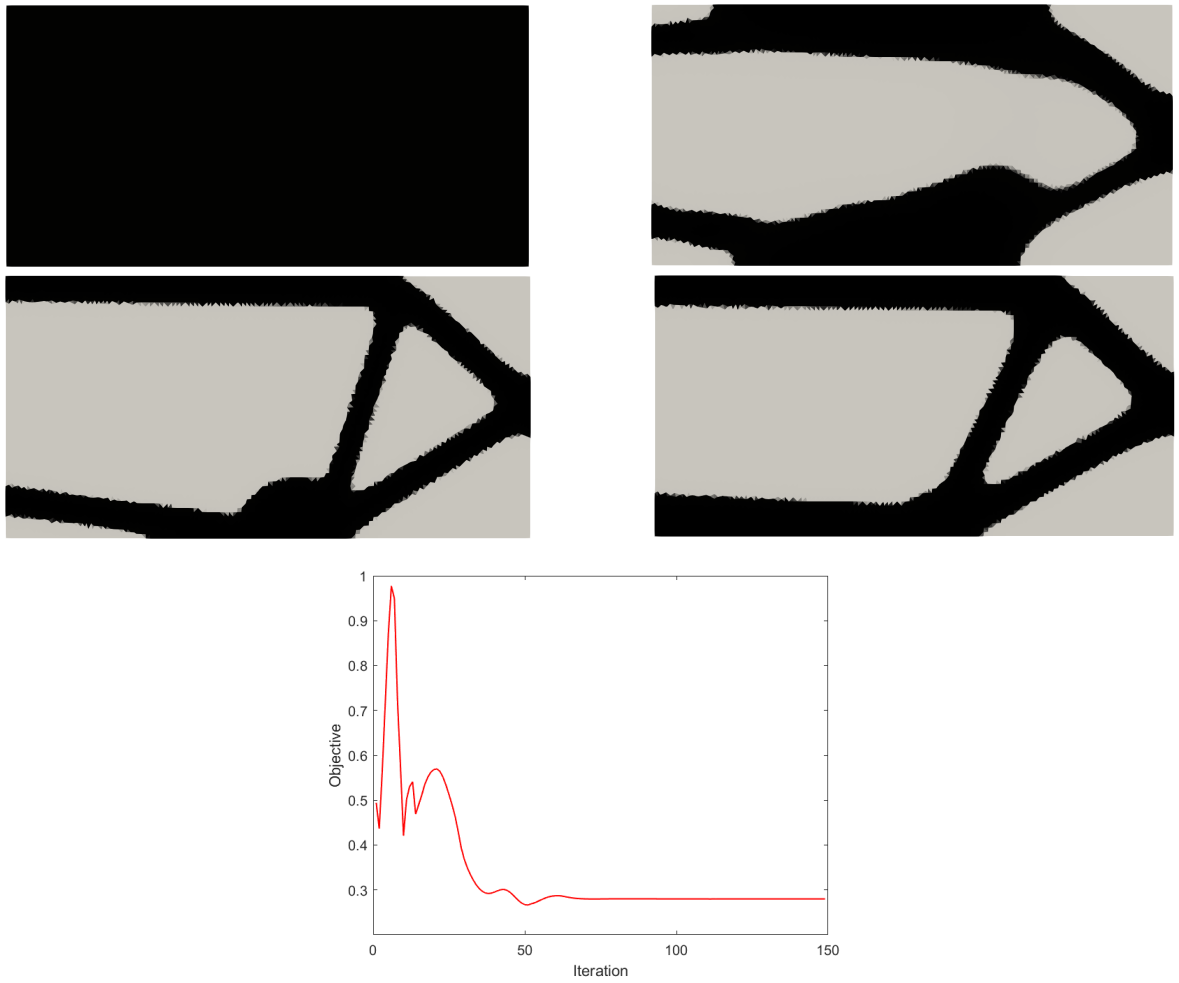


Figure 3.12: shape optimization using level set method with topological derivative.

unchanged. The choice of the initial phase field is the same as in example 3.2.2, as shown in Figure 3.7b

As in the previous numerical example, in this example, we incorporate the effects of topological sensitivity into the phase evolution equations. This is achieved by adding a term driven by the topological derivative $\mathcal{T}(x)$ in the Allen-Cahn dynamics.

The evolution process is shown in Figure 3.13. The convergence history of the objective function is shown in Figure 3.14, where the objective function eventually flattens out as the number of iterations increases, i.e., converges.

This example demonstrates the advantage of combining the phase field method with topological derivatives: the topological term provides global sensitivity information, which enables more efficient navigation of the design space, especially in complex mechanical environments with contact constraints.

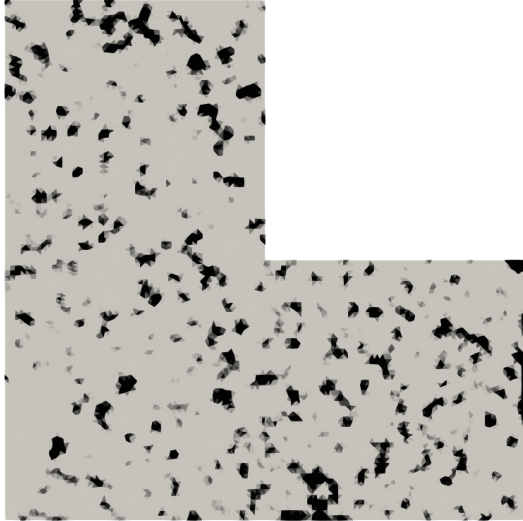
Example 3.2.5. In this example, we extend the proposed phase field-topological derivative method to a three-dimensional structural optimization problem under a single-sided contact constraint. The purpose is to demonstrate the ability of the method to handle high-dimensional complex topological changes.

The design domain is defined as a cuboid $D = [0, 2] \times [0, 1] \times [0, 1]$. The left side of the domain (i.e., $\{0\} \times [0, 1] \times [0, 1]$) is clamped, while a uniform downward vertical load is applied to the central region of the right side. A small portion of the center of the bottom surface is modeled as a rigid obstacle, and a single-sided contact condition governed by a Signorini-type inequality is introduced.

The initial phase field $\varphi_0(x)$ is taken as a smooth random distribution with support inside D , as shown in Figure 3.15b. The optimization process is performed via the Allen-Cahn gradient flow, and the topological derivative term $\mathcal{T}(x)$ is added.

The final results of the phase field and topology over iterations are shown in Fig. 3.15, where the isosurface rendering of $\varphi \approx 0$ reveals the emerging structural features. The design starts with scattered material fragments that gradually merge and reshape into a load-bearing structure while responding to contact constraints.

Fig. 3.16 plots the convergence of the objective function, demonstrating the effectiveness of the optimization process. The final structure exhibits good load path connectivity and avoids penetrating obstacles, validating the three-dimensional scalability of our method.



(a) Iteration 10



(b) Iteration 50



(c) Iteration 100



(d) Final design

Figure 3.13: Shape optimization process for Example 3.2.4: Snapshots of the phase field at selected iterations.

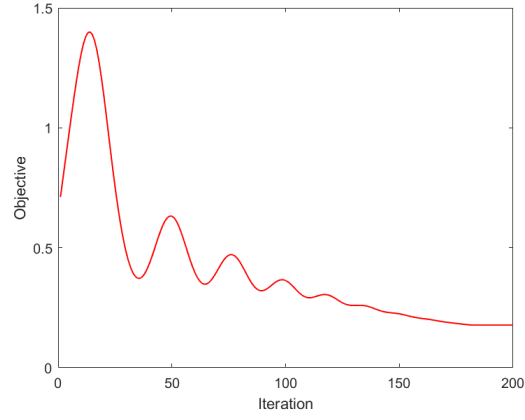
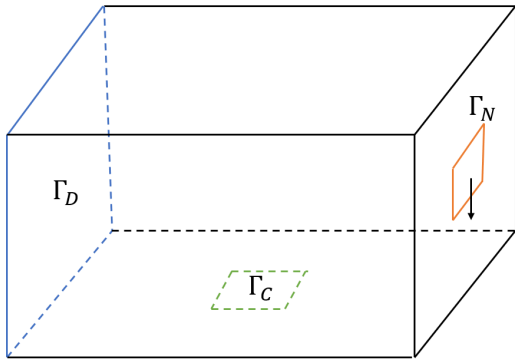
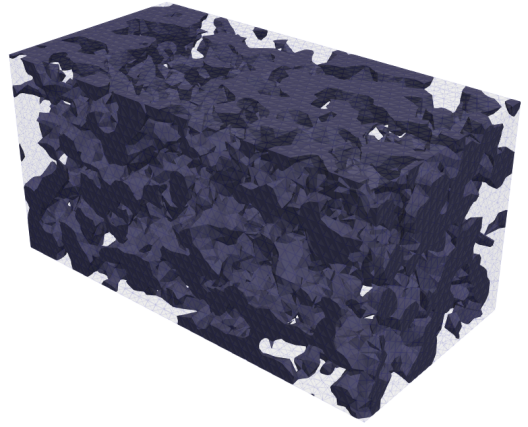


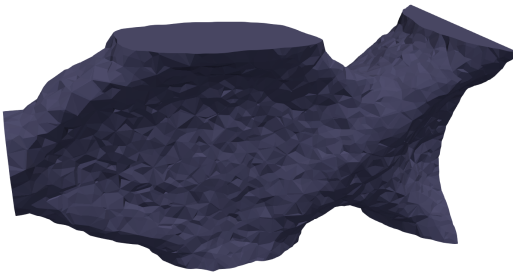
Figure 3.14: Convergence history of the objective function for Example 3.2.4.



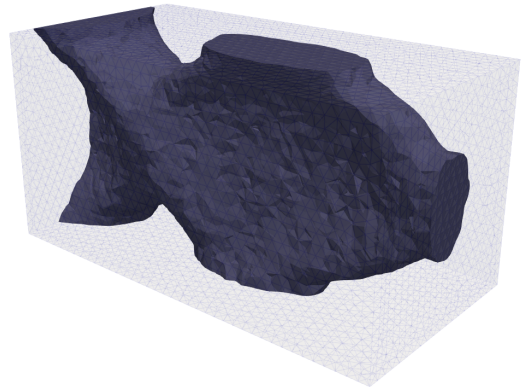
(a) Model setup



(b) Initial phase field



(c) Final design



(d) Final design

Figure 3.15: Phase field evolution for Example 3.2.5 at selected iterations.

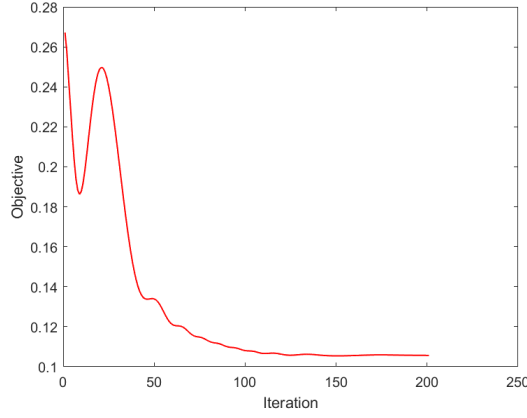


Figure 3.16: Objective function convergence history for Example 3.2.5.

3.3 Contact problem with friction

After completing the systematic study of the frictionless contact (Signorini) problem, we have fully mastered the deformation behavior of elastic bodies under unilateral constraints and its mathematical modeling framework. However, in many practical engineering applications, the contact interface not only has normal constraints, but also is accompanied by significant tangential friction effects, which significantly affect the stress transfer and response mode of the structure. Therefore, in order to be closer to physical reality and expand the applicability of the model, the next work will further study the contact problem with friction.

In the study of contact problems in elastic materials, the sliding contact model represents one of the fundamental formulations, particularly relevant for scenarios where no friction is present. It builds upon the classical Signorini framework, with an important refinement: it imposes zero tangential stress on the contact interface. This addition makes the model suitable for describing frictionless sliding, not only in a conceptual sense but also in a mathematically precise and physically realistic manner. The sliding contact model is commonly applied in engineering contexts such as light or intermittent contact between structural components, smooth interactions in mechanical assemblies, or self-contact phenomena as seen in crack closure or folded materials. Although the deformation of the structure is assumed to be small—making the use of linearised elasticity theory appropriate—the introduction of contact constraints fundamentally alters the character of the problem, introducing nonlinear boundary conditions and unknown contact regions. These features significantly increase the mathematical and computational complexity, necessitating special analytical tools and numerical strategies.

In a standard setting, the domain occupied by the elastic body is denoted by $\Omega \subset \mathbb{R}^d$, where $d = 2$ or 3 . The boundary $\partial\Omega$ is partitioned into five disjoint parts: Γ_0 is the clamped boundary, where displacement is fixed to zero; Γ_N is the Neumann boundary, where external surface forces g are prescribed; Γ denotes the free boundary with no prescribed forces or displacements; Γ_C is a potential contact boundary with a rigid obstacle; and S is an internal surface where self-contact may occur (for instance, in the case of a crack or material fold). The central assumption of the sliding contact model is that when contact occurs, tangential movement is permitted without resistance—i.e., friction is neglected. This assumption not only reflects many realistic physical systems but also allows for a more tractable mathematical formulation.

Mathematically, the contact boundary conditions on Γ_C are composed of three principal components that describe the normal interaction between the structure and the obstacle. First is the non-penetration condition, ensuring that the structure does not pass through the obstacle. It is expressed as:

$$\mathbf{u} \cdot \mathbf{n} \leq 0, \quad (3.124)$$

where n is the unit outward normal on Γ_C , and u is the displacement vector field. Second, the compressive normal stress condition ensures that contact pressure (if present) is pushing the structure inward rather than pulling it away:

$$(A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n}) \cdot \mathbf{n} \leq 0. \quad (3.125)$$

Third, the complementarity condition enforces that contact force appears if and only if the structure is in contact:

$$(\mathbf{u} \cdot \mathbf{n})(A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n}) \cdot \mathbf{n} = 0. \quad (3.126)$$

This framework, collectively known as the Signorini conditions, guarantees that the system correctly models unilateral, frictionless contact. That is, contact occurs only under compression, never under tension, and only at locations where the body actually touches the obstacle.

Given the assumption of frictionless behavior, the tangential stress must also vanish on the contact interface. This is a key distinction between the sliding contact model and the classical Signorini formulation. It is expressed mathematically as:

$$(A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n})_t = 0, \quad (3.127)$$

where $(\cdot)_t$ denotes the tangential component of a vector with respect to the boundary surface. This constraint eliminates shear forces on the interface and ensures that, in the

presence of contact, the interface behaves as a perfectly smooth surface. Importantly, this condition is imposed not only on the external contact boundary Γ_C , but also on both sides of the internal self-contact surface S , namely on S_- and S_+ . This reflects the model's consistency in both external and internal contact situations, ensuring no tangential traction is transmitted across any contact interface.

For the self-contact interface S , the sliding contact conditions are more naturally expressed using jump notation. Specifically, the displacement jump across S is defined as:

$$[\mathbf{u}] = \mathbf{u}|_{S_-} - \mathbf{u}|_{S_+}, \quad (3.128)$$

where S_- and S_+ denote the two sides of the interface, and $\mathbf{n}_-$ is the unit normal on S_- pointing toward S_+ . The sliding self-contact conditions mirror the boundary contact case in both structure and spirit. First, the non-penetration across S is expressed as:

$$[\mathbf{u}] \cdot \mathbf{n}_- \leq 0. \quad (3.129)$$

Second, the compressive stress condition is enforced symmetrically:

$$A\boldsymbol{\varepsilon}(\mathbf{u}|_{S_-})\mathbf{n}_- \cdot \mathbf{n}_- = A\boldsymbol{\varepsilon}(\mathbf{u}|_{S_+})\mathbf{n}_- \cdot \mathbf{n}_- \leq 0. \quad (3.130)$$

Third, the complementarity condition for self-contact is given by:

$$([\mathbf{u}] \cdot \mathbf{n}_-)(A\boldsymbol{\varepsilon}(\mathbf{u}|_{S_-})\mathbf{n}_- \cdot \mathbf{n}_-) = 0. \quad (3.131)$$

Together, these conditions ensure that no material interpenetration occurs across S , that normal contact stresses are continuous and compressive, and that such stresses are only nonzero where actual contact takes place.

To rigorously treat these nonlinear boundary conditions, the sliding contact problem is cast within the framework of variational inequalities. One begins by defining the space of admissible displacement fields. Let $H_{\Gamma_0}^1(\Omega)^d$ denote the Sobolev space of vector-valued functions that vanish on the clamped portion Γ_0 of the boundary. Then define the admissible set:

$$K(\Omega) = \{\mathbf{v} \in H_{\Gamma_0}^1(\Omega)^d \mid \mathbf{v} \cdot \mathbf{n} \leq 0 \text{ on } \Gamma_C, [\mathbf{v}] \cdot \mathbf{n}_- \leq 0 \text{ on } S\}. \quad (3.132)$$

This set encodes the unilateral contact constraints in both the external and internal contact regions. The weak formulation of the sliding contact problem then seeks a solution $\mathbf{u} \in K(\Omega)$ such that:

$$\int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u} - \mathbf{v}) \, dx \geq \int_{\Omega} \mathbf{f} \cdot (\mathbf{u} - \mathbf{v}) \, dx + \int_{\Gamma_N} \mathbf{g} \cdot (\mathbf{u} - \mathbf{v}) \, ds \quad \forall \mathbf{v} \in K(\Omega), \quad (3.133)$$

where $f \in L^2(\Omega)^d$ and $g \in L^2(\Gamma_N)^d$ denote the volume force and surface traction, respectively. This variational inequality captures both the mechanical equilibrium of the elastic structure and the non-penetration and complementarity conditions inherent in the sliding contact framework.

Importantly, this variational inequality is not just a convenient mathematical abstraction. It is equivalent to the Euler–Lagrange optimality condition of a constrained energy minimisation problem, which seeks the displacement field $\mathbf{u}$ that minimizes the total potential energy of the system, subject to the unilateral constraints. The minimisation problem is:

$$\mathbf{u} = \operatorname{argmin}_{\mathbf{v} \in K(\Omega)} \left[\frac{1}{2} \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{v}) : \boldsymbol{\varepsilon}(\mathbf{v}) \, dx - \int_{\Omega} f \cdot \mathbf{v} \, dx - \int_{\Gamma_N} P \cdot \mathbf{v} \, ds \right]. \quad (3.134)$$

3.3.1 Contact problems with Tresca friction

In solid mechanics, contact problems with friction concern the behavior of deformable bodies that come into contact under the influence of external forces, while taking into account the effects of friction. These problems are ubiquitous in engineering and applied physics, such as in tire–road interaction, gear meshing, and metal forming processes. The core challenge lies in accurately modeling the interaction forces—particularly the coupling between normal contact forces and tangential frictional forces.

When two elastic bodies are in contact, the normal contact force prevents interpenetration, while the friction force resists relative tangential motion. The modeling of friction is a critical aspect, as different friction laws yield significantly different physical predictions. Commonly used friction models include the Coulomb model, the Tresca model, and various regularized or smooth approximations of these.

Mathematically, contact problems with friction are inherently nonlinear and non-smooth, especially due to the threshold behavior that distinguishes sticking from sliding. As a result, these problems cannot be treated using classical linear elasticity and are instead formulated as variational inequalities or quasi-variational inequalities, allowing the use of tools from convex analysis and functional analysis for both theoretical and numerical treatment.

Let u denote the displacement field of the deformable body. The normal contact conditions ensure non-penetration at the contact interface, while the friction conditions impose bounds on the tangential stress component $(A\boldsymbol{\varepsilon}(\mathbf{u})\mathbf{n})_t$, regulating sliding behavior. The governing system must satisfy both the elasticity equations and the friction laws prescribed on the contact boundary.

The study of contact problems with friction is not only of theoretical interest but also of substantial practical relevance. It provides the mathematical foundation and computational tools for analyzing complex interface mechanics, predicting structural response under frictional contact, and enabling robust optimization in mechanical design.

3.3.2 Tresca friction model

In the study of elastic contact problems, the introduction of friction transforms the problem from a classical linear boundary value formulation into a nonlinear and non-smooth system. When relative tangential motion occurs at the contact interface, the frictional force plays a crucial role in regulating and constraining the sliding behavior. To model such frictional effects, appropriate constitutive relations must be imposed along the contact boundary. Among various models, the Tresca friction model is widely used due to its structural simplicity and favorable mathematical properties, especially in the context of nonsmooth variational formulations and finite element implementations.

The core idea of the Tresca model is to prescribe an upper bound on the tangential stress at the contact interface. This bound is given by a position-dependent function $\sigma_{\text{tr}}(x)$, commonly referred to as the friction threshold or friction limit. This threshold is typically assumed to be nonnegative and continuous, and it reflects surface characteristics of the material or lubrication conditions. The model posits that when the norm of the tangential contact stress σ_t is strictly less than the friction threshold, the interface remains in a state of sticking with no relative slip. Once the tangential stress reaches the threshold, sliding may occur in a direction opposite to that of the tangential stress vector, thus giving rise to a nonsmooth but physically interpretable boundary condition.

Let $\Omega \subset \mathbb{R}^d$ be the reference configuration of the elastic body, where $d = 2$ or 3 . The boundary $\partial\Omega$ is decomposed into three disjoint parts: the Dirichlet boundary Γ_D , the Neumann boundary Γ_N , and the potential contact boundary Γ_C , i.e.,

$$\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_C, \quad \Gamma_D \cap \Gamma_N = \Gamma_D \cap \Gamma_C = \Gamma_N \cap \Gamma_C = \emptyset. \quad (3.135)$$

The displacement field $\mathbf{u} : \Omega \rightarrow \mathbb{R}^d$ satisfies the linearized strain tensor under small deformation assumptions, defined by

$$\boldsymbol{\varepsilon}(\mathbf{u}) := \frac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^\top).$$

The stress tensor follows the linear isotropic elasticity law

$$\boldsymbol{\sigma}(\mathbf{u}) = A\boldsymbol{\varepsilon}(\mathbf{u}),$$

where A is a fourth-order, symmetric, and positive-definite elasticity tensor satisfying the uniform ellipticity condition. The outward unit normal on the contact boundary Γ_C is denoted by $\mathbf{n}(x)$, and the tangential projection of a vector $\mathbf{v}$ is given by

$$\mathbf{v}_t := \mathbf{v} - (\mathbf{v} \cdot \mathbf{n})\mathbf{n}.$$

Accordingly, the tangential component of the stress vector is defined as

$$\boldsymbol{\sigma}_t := \boldsymbol{\sigma}(\mathbf{u})\mathbf{n} - (\boldsymbol{\sigma}(\mathbf{u})\mathbf{n} \cdot \mathbf{n})\mathbf{n}.$$

The Tresca friction law on Γ_C is characterized by the following conditions for each point $x \in \Gamma_C$:

- If $\|\boldsymbol{\sigma}_t(x)\| < \boldsymbol{\sigma}_{\text{tr}}(x)$, then the interface is in sticking contact, and $\mathbf{u}_t(x) = 0$;
- If $\|\boldsymbol{\sigma}_t(x)\| = \boldsymbol{\sigma}_{\text{tr}}(x)$, then sliding may occur, and there exists a nonnegative scalar function $\lambda(x) \geq 0$ such that $\mathbf{u}_t(x) = -\lambda(x)\boldsymbol{\sigma}_t(x)$;
- The unified condition is $\|\boldsymbol{\sigma}_t(x)\| \leq \boldsymbol{\sigma}_{\text{tr}}(x)$, implying that the tangential stress remains bounded by the friction threshold.

This model essentially imposes a constraint on the norm of the tangential stress, which can be interpreted as a set-valued relation between tangential stress and displacement. From a variational standpoint, the problem can be reformulated in terms of an inequality or minimization problem. The frictional functional $j_{\text{tr}} : H^1(\Omega; \mathbb{R}^d) \rightarrow \mathbb{R}_+$ is introduced as

$$j_{\text{tr}}(\mathbf{v}) := \int_{\Gamma_C} \boldsymbol{\sigma}_{\text{tr}}(x) \|\mathbf{v}_t(x)\| ds, \quad (3.136)$$

representing the energy dissipation or penalty associated with tangential displacement at the contact interface.

The elastic contact problem under Tresca friction then leads to the following variational inequality: find $\mathbf{u} \in K$ such that

$$\int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{u} - \mathbf{v}) dx + j_{\text{tr}}(\mathbf{v}) - j_{\text{tr}}(\mathbf{u}) \geq \int_{\Omega} \mathbf{f} \cdot (\mathbf{u} - \mathbf{v}) dx + \int_{\Gamma_N} \mathbf{P} \cdot (\mathbf{u} - \mathbf{v}) ds, \quad \forall \mathbf{v} \in K, \quad (3.137)$$

where f denotes the volume force and g the surface traction on the Neumann boundary. This inequality characterizes the equilibrium state of the system under external loads, contact constraints, and frictional interaction.

Equivalently, the problem can be recast as a nonsmooth convex minimization problem:

$$\mathbf{u} = \operatorname{argmin}_{\mathbf{v} \in K} \left\{ \frac{1}{2} \int_{\Omega} A \boldsymbol{\varepsilon}(\mathbf{v}) : \boldsymbol{\varepsilon}(\mathbf{v}) \, dx - \int_{\Omega} f \cdot \mathbf{v} \, dx - \int_{\Gamma_N} P \cdot \mathbf{v} \, ds + j_{\text{tr}}(\mathbf{v}) \right\}, \quad (3.138)$$

which consists of a strongly convex quadratic energy functional combined with a convex, positively homogeneous, nonsmooth term representing the friction. Due to the strong convexity of the elastic energy and the continuity and convexity of the friction functional, this minimization problem admits a unique solution under standard assumptions. The solution corresponds to the mechanical equilibrium configuration of the body under Tresca-type frictional constraints.

Regularization of the Friction Term

In the frictional contact models, including the Tresca model discussed previously, the use of the norm $|\cdot|$ in the tangential stress constraints leads to non-smooth variational inequalities. To reformulate the problem into a smooth and differentiable setting suitable for numerical optimization, we regularize the norm using a smooth approximation.

Let $\mathcal{N}_\eta : \mathbb{R}^d \rightarrow \mathbb{R}$ be a twice continuously differentiable (C^2) approximation of the Euclidean norm. A common choice, as proposed in Eck et al., 2005, is:

$$\mathcal{N}_\eta(x) = \begin{cases} \|x\|, & \text{if } \|x\| \geq \eta, \\ -\frac{1}{8\eta^3} \|x\|^4 + \frac{3}{4\eta} \|x\|^2 + \frac{3}{8}\eta, & \text{if } \|x\| \leq \eta, \end{cases} \quad (3.139)$$

where $\eta > 0$ is a small smoothing parameter that defines the transition region near zero.

Under this regularization, the smoothed Tresca friction energy functional becomes:

$$j_{\text{tr},\eta}(\mathbf{v}) := \int_{\Gamma_C} \sigma_{\text{tr}}(x) \mathcal{N}_\eta(\mathbf{v}_t(x)) \, ds + \int_S \sigma_{\text{tr}}(x) \mathcal{N}_\eta([\mathbf{v}]_t(x)) \, ds, \quad (3.140)$$

where $\mathbf{v}_t$ denotes the tangential component of $\mathbf{v}$ on Γ_C , and $[\mathbf{v}]_t$ denotes the tangential jump of $\mathbf{v}$ across the self-contact surface S .

To enforce non-penetration conditions $\mathbf{v} \cdot \mathbf{n} \leq 0$ on Γ_C (and possibly on S), we introduce a penalization term $j_{N,\epsilon}(\mathbf{v})$, such as a quadratic or logarithmic barrier functional. The explicit form of $j_{N,\epsilon}$ can vary depending on the chosen penalization strategy and is omitted here for brevity.

With these modifications, the regularized and penalized variational form of the Tresca friction contact problem reads:

$$\int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) dx + j'_{\text{tr},\eta}(\mathbf{u}, \mathbf{v}) + j'_{N,\epsilon}(\mathbf{u}, \mathbf{v}) = \int_{\Omega} f \cdot \mathbf{v} dx + \int_{\Gamma_N} P \cdot \mathbf{v} ds, \quad \forall \mathbf{v} \in H_{\Gamma_0}^1(\Omega)^d, \quad (3.141)$$

where $j'_{\text{tr},\eta}(\mathbf{u}, \mathbf{v})$ and $j'_{N,\epsilon}(\mathbf{u}, \mathbf{v})$ are the directional derivatives of the respective regularized functionals.

Equivalently, the problem can be formulated as a smooth convex minimization problem:

$$\mathbf{u} = \underset{v \in H_{\Gamma_0}^1(\Omega)^d}{\operatorname{argmin}} \left\{ \frac{1}{2} \int_{\Omega} A\boldsymbol{\varepsilon}(\mathbf{v}) : \boldsymbol{\varepsilon}(\mathbf{v}) dx - \int_{\Omega} f \cdot \mathbf{v} dx - \int_{\Gamma_N} P \cdot \mathbf{v} ds + j_{N,\epsilon}(\mathbf{v}) + j_{\text{tr},\eta}(\mathbf{v}) \right\}. \quad (3.142)$$

This formulation preserves the key features of the Tresca friction law while enabling efficient numerical treatment using gradient-based optimization methods or smooth finite element solvers. Importantly, such a regularization approach yields a well-posed, convex, and differentiable optimization problem that admits a unique solution under standard assumptions.

Theorem 3.3.1. *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain and the displacement field $\mathbf{u} = \mathbf{u}[\varphi] \in H_{\Gamma_0}^1(\Omega)^d$ be the unique solution of the variational inequality on $\Gamma_C \cup S$ with regularized Tresca friction. The Euler derivative of the compliance-type functional:*

$$\mathcal{J}(\varphi) := \int_{\Omega} f \cdot \mathbf{u}[\varphi] dx \quad (3.143)$$

in direction $\delta\varphi \in C_c^\infty(D)$ is given by

$$\delta\mathcal{J}(\varphi)[\delta\varphi] = -\frac{1}{2} \int_{\Omega} \chi'(\varphi)(A_1 - A_0)\boldsymbol{\varepsilon}(\mathbf{u}[\varphi]) : \boldsymbol{\varepsilon}(\mathbf{p}[\varphi]) \delta\varphi dx, \quad (3.144)$$

where $\mathbf{p} = \mathbf{p}[\varphi] \in H_{\Gamma_0}^1(\Omega)^d$ is the solution to the following adjoint variational inequality:

Find $\mathbf{p} \in K(0) := \{\mathbf{v} \in H_{\Gamma_0}^1(\Omega)^d \mid \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \Gamma_c, [\mathbf{v}] \cdot \mathbf{n} = 0 \text{ on } S\}$ such that:

$$\int_{\Omega} A(\varphi)\boldsymbol{\varepsilon}(\mathbf{p}) : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{p}) dx + \delta j'_{\text{tr},\eta}(\mathbf{u}; \mathbf{v} - \mathbf{p}) \geq \int_{\Omega} f \cdot (\mathbf{v} - \mathbf{p}) dx \quad \forall \mathbf{v} \in K(0). \quad (3.145)$$

Proof. We aim to compute the shape derivative (Euler derivative) of the functional:

$$\mathcal{J}(\varphi) := \int_{\Omega} f \cdot \mathbf{u}[\varphi] dx. \quad (3.146)$$

Note that the functional depends on φ only through the state variable $\mathbf{u}[\varphi]$, which itself is the solution to a nonlinear variational inequality constrained by regularized frictional contact. The dependence is thus implicit.

We proceed using the chain rule:

$$\delta\mathcal{J}(\varphi)[\delta\varphi] = \int_{\Omega} f \cdot \delta\mathbf{u}[\delta\varphi] dx, \quad (3.147)$$

where $\delta\mathbf{u} \in H_{\Gamma_0}^1(\Omega)^d$ is the material derivative of the solution $\mathbf{u}[\varphi]$ in the direction $\delta\varphi$. Since $\mathbf{u}$ solves a variational inequality, $\delta\mathbf{u}$ satisfies a generalized directional differentiability condition, and we apply an adjoint method.

Let $\mathbf{p} \in H_{\Gamma_0}^1(\Omega)^d$ solve the adjoint variational inequality:

$$\int_{\Omega} A(\varphi)\boldsymbol{\varepsilon}(\mathbf{p}) : \boldsymbol{\varepsilon}(\mathbf{v} - \mathbf{p}) dx + \delta j'_{\text{tr},\eta}(\mathbf{u}; \mathbf{v} - \mathbf{p}) \geq \int_{\Omega} f \cdot (\mathbf{v} - \mathbf{p}) dx, \quad \forall \mathbf{v} \in K(0). \quad (3.148)$$

From variational inequality sensitivity theory, we can formally express the directional derivative of u in direction $\delta\varphi$ as satisfying:

$$\int_{\Omega} A(\varphi)\boldsymbol{\varepsilon}(\delta\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) dx + \delta j'_{\text{tr},\eta}(\mathbf{u}; \mathbf{v}) = - \int_{\Omega} A'(\varphi)[\delta\varphi]\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) dx, \quad \forall \mathbf{v} \in K(0), \quad (3.149)$$

where $A'(\varphi)[\delta\varphi] = \chi'(\varphi)(A_1 - A_0)\delta\varphi$. Testing this equation with the adjoint variable p , and using the definition of $\delta\mathcal{J}(\varphi)$, we obtain:

$$\delta\mathcal{J}(\varphi)[\delta\varphi] = \int_{\Omega} f \cdot \delta\mathbf{u} dx = - \int_{\Omega} \chi'(\varphi)(A_1 - A_0)\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{p})\delta\varphi dx. \quad (3.150)$$

Finally, since A is symmetric and χ' is scalar, we symmetrize:

$$\delta\mathcal{J}(\varphi)[\delta\varphi] = -\frac{1}{2} \int_{\Omega} \chi'(\varphi)(A_1 - A_0)\boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{p})\delta\varphi dx. \quad (3.151)$$

This completes the proof. □

3.3.3 Numerical examples

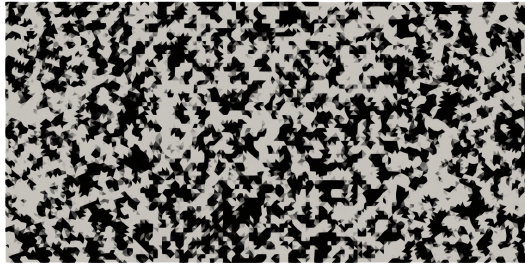
Example 3.3.1. *In this example, we extend the previous benchmark setup by introducing frictional contact and modeling it using the regularized Tresca friction law. The geometric and mechanical setup is the same as in example 3.2.1, with a computational domain of $D = [0, 2] \times [0, 2]$, fixed boundary conditions at the left edge, and a vertical load at the center of the right boundary. The center portion of the bottom boundary*

acts as a potential contact interface, but unlike the frictionless Signorini case, we now introduce a tangential drag via a Tresca-type condition.

The optimization is performed using the phase field method, where the material distribution is controlled by a smoothed scalar field $\varphi \in H^1(D)$ that evolves under an Allen-Cahn-type gradient flow. The total energy functional includes contributions from the elastic compliance, the regularized interface energy, and the frictional contact. The state variable $u = u[\varphi]$ satisfies a regularized variational inequality at each iteration that accounts for both normal and tangential contact effects.

The initial phase field φ_0 is set to a smooth random distribution (see Figure 3.17a). As the optimization proceeds, the interface evolves and the algorithm refines the material topology while satisfying the single-sided contact and friction constraints. Figure 3.17 shows the intermediate phase field configurations after the selected number of iterations, and the final design is shown in Figure 3.17d.

The convergence history of the compliance function, as shown in Figure 3.18, shows that the energy eventually converges to a stable configuration. Figure 3.5a shows the problem setup, including loads and boundary conditions, as a schematic for reference.



(a) Initial phase field



(b) Iteration 20



(c) Iteration 50



(d) Final design

Figure 3.17: Shape optimization process for Example 3.3.1 with Tresca friction. Sub-figures show the phase field evolution at selected iterations.

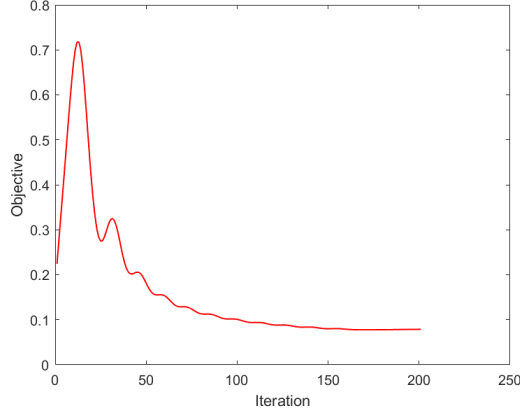


Figure 3.18: Objective function convergence history for Example 3.3.1.

Example 3.3.2. *In this example, we extend the 2D benchmark to a 3D environment while keeping the same physical model, which involves frictional contact and phase-field-based structural optimization following the regularized Tresca's law.*

The computational domain is defined as a cube $D = [0, 2] \times [0, 2] \times [0, 2]$ from which a smaller subdomain $[0, 1] \times [1, 2] \times [0, 1]$ is removed, resulting in an inverted L-shaped structure. Dirichlet boundary conditions are applied to the left face $\Gamma_D = [0, 2] \times \{0\} \times [0, 2]$ enforcing fixed displacements. A vertical downward load is applied to the top center portion of the domain, defined as $\Gamma_N = [0.8, 1.2] \times \{2\} \times [0.8, 1.2]$. The contact interface Γ_C is located on the bottom center surface $[0.8, 1.2] \times [0.8, 1.2] \times \{0\}$, where the friction contact is controlled by the regularized Tresca condition as shown in Figure. 3.19.

The material distribution is controlled by the phase field variables $\varphi \in H^1(D)$ which evolve via an Allen-Cahn type gradient flow. The optimization problem is to minimize the total energy function that includes the elastic compliance, the regularized interface energy, and the friction contact contribution. The state variables $u = u[\varphi]$ satisfy the regularized variational inequality that considers both the normal contact force and the tangential friction force at each iteration.

The initial phase field φ_0 is initialized as a smooth random field (see Figure 3.19). During the optimization process, the material layout evolves to adapt to the loads and contact conditions. The final optimized structure is shown in Figure 3.20.

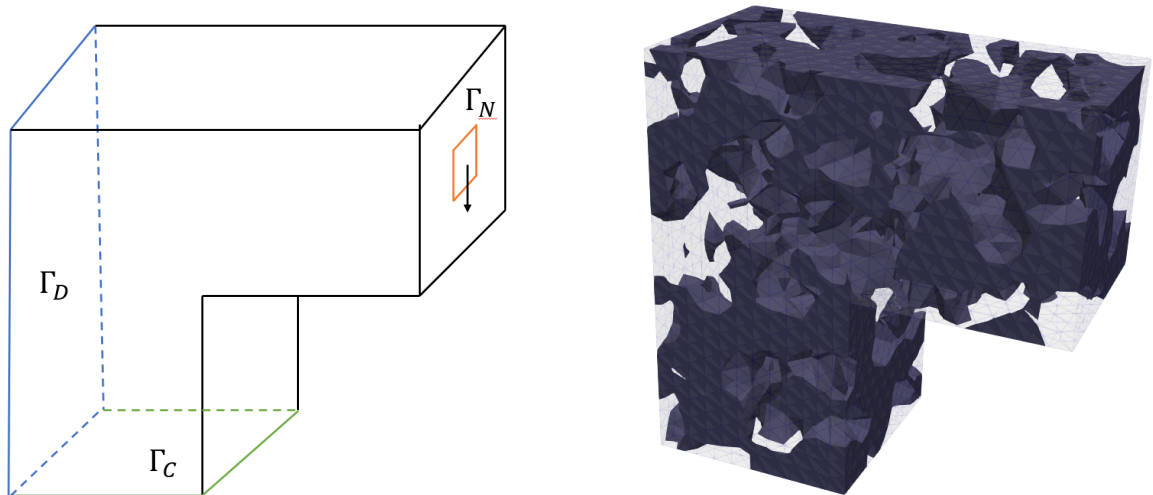


Figure 3.19: Model setup and initial phase field for Example. 3.3.2



Figure 3.20: The Final result of Example. 3.3.2

Chapter 4

Gradient Flow in Shape Optimization

Having solved shape and topology optimization problems under contact constraints in the phase field framework (ranging from the classical Signorini conditions to the more advanced Tresca-type friction laws), we will now turn to a different but related class of approaches, rooted in the theory of gradient flows. Gradient flows in shape optimization with partial differential equation (PDE) constraints is an emerging research area in the field of partial differential equations (PDEs). P.I. Plotnikov and J. Sokolowski have published three papers on this topic. The authors' forthcoming monograph will provide a complete proof of the existence of solutions of the gradient flow system in two models. The first model is the inverse problem for the Laplace operator. The second model is the well-known Bernoulli free boundary problem. The relevant shape functionals to be minimized are of the Kohn-Vogelius type. This means that the Hadamard shape gradients of such functionals are defined in terms of the solutions to the elliptic problem, without the need to compute adjoint states. Shape optimization problems for the Laplace operator and linear elasticity are considered in this chapter. The numerical results reported in this chapter are new. Our calculations confirm the abstract theory. The Willmore functional is used to regularize the considered shape optimization problem. The resulting quasi-linear dynamical system is numerically solved using an explicit format, so this method is slow and requires many iterations.

4.1 Overview of shape optimization theory

Shape optimization is a mathematical field situated at the intersection of the calculus of variations and free boundary problems. It was systematically developed as an independent discipline in the foundational monographs Delfour and Zolésio, 2011a; Sokolowski and Zolesio, 1992. Over the past few decades, it has evolved into a robust theory with applications in distributed control systems, structural mechanics, transportation networks, free boundary problems, and inverse problems in numerical analysis.

In shape optimization there are two main theoretical problems in the continuous setting:

1. The existence of optimal shapes;
2. The convergence of numerical method for solution of shape optimization problem.

The latter topic is new and leads to difficult mathematical questions. In the continuous setting the Gradient Flow Dynamical System for shape optimization (GFDS) is introduced and studied in the recent publications Plotnikov and Sokolowski, 2023a, Plotnikov and Sokolowski, 2023c, Plotnikov and Sokolowski, 2023b as well as in the forthcoming book by the same authors entitled *Geometric Framework for Gradient Flow in Shape Optimization* to appear in SpringerBriefs, PDEs and Data Science. The theory in this chapter for the scalar problems is presented for the convenience of the reader and it is borrowed from the book. It is shown in the book that (GFDS) admit solutions for two model problems. The first is an inverse problem with the Kohn-Vogelius type cost. The second is the Bernoulli free boundary problem.

The proof of convergence of the simple gradient method in the continuous form of (GFDS) is performed in the book by using the new variant of the famous Nash-Moser iterative scheme which is nothing else as the Newton method with smoothing. The results of dissertation which are obtained for linearized elasticity are new.

The theoretical results from the above book are repeated (see Theorem 2.5) for the purposes of numerical methods in Dissertation. The numerical methods are new and it is an original and important contribution of Dissertation to the field of Shape Optimization. Our results confirm that the (GFDS) dynamical system is a new and efficient tool in resolution of optimality conditions in shape optimization. The results are restricted to $2D$ PDEs, the general case of $3D$ PDEs is an open and difficult problem.

In the Dissertations we present many examples of numerical solution for the system (GFDS). The new examples are presented for linear elasticity and the unilateral contact

problems. Our results confirm the general theory as well as open to the mathematical analysis the important applications e.g., in linearized elasticity.

A widely used approach involves formulating shape optimization problems as dynamical systems, where Newton-type methods combined with smoothing techniques are employed to solve inverse problems. The Nash-Moser iteration scheme provides a framework for analyzing global convergence, particularly in infinite-dimensional settings. Recent progress has established the convergence of steepest descent methods in this context, opening new directions for theoretical and numerical research. Simplified model problems—such as compliance minimization—are often used to demonstrate the feasibility and adaptability of these techniques.

Shape optimization is typically framed on a fixed domain D , where variable subdomains $\Omega \subset D$ are analyzed. The governing state equations are usually partial differential equations (PDEs), which may be elliptic, parabolic, or hyperbolic, or nonlinear systems arising from fluid or solid mechanics. The objective is to minimize a cost functional $J(\Omega)$, which evaluates the performance of the domain. To guide the optimization, shape sensitivity analysis provides expressions for the first- and second-order derivatives of $J(\Omega)$ using the velocity method, leading to shape gradients and Hessians that are crucial for algorithmic implementation.

In recent years, gradient flow methods have gained attention as an alternative and effective framework. These methods recast shape optimization as an evolution process, where the domain evolves continuously along the direction of steepest descent of the cost functional. The shape propagates with a velocity field defined by the gradient, ensuring a monotonic decrease in cost. This approach not only provides an intuitive geometric interpretation but also naturally accommodates constraints and nonlinearities. Theoretical results have established existence, uniqueness, and convergence of such flows in various settings, as detailed in Plotnikov and Sokolowski, 2023a, 2023b; Plotnikov and Sokolowski, 2023c. Consequently, gradient flows have significantly enhanced the robustness and efficiency of numerical optimization schemes.

Shape optimization also plays a crucial role in inverse problems, where the goal is to reconstruct domain shapes based on observed data. Adjusting shapes to fit measurements improves both the stability and accuracy of the solutions. The existence of optimal shapes has been rigorously studied in Allen and Cahn, 1979; Calisti et al., 2023; Tan and Zhu, 2024. In the context of multiscale structural design Ganghoffer, Goda, et al., 2018; Giusti et al., 2019, homogenization methods are widely used to handle material distribution at fine scales. Moreover, topological derivative methods

have expanded the field to include topology optimization, which involves modifying not just the boundaries but also the connectivity and material layout within the domain, as shown in Bendsøe and Sigmund, 2004; Kazmierczak et al., 2018; Leugering et al., 2022; Novotny et al., 2019a, 2019b, 2019c.

Through the integration of advanced mathematical tools and computational techniques, shape optimization continues to advance both theoretically and practically, with a growing impact across engineering, physics, and data science.

4.2 Geometric foundations for curve-based shape optimization

Let $\Omega \subset \mathbb{R}^2$ be a smooth, bounded domain, and consider a family of smooth Jordan curves $\Gamma \Subset \Omega$, each of class C^∞ . Every such curve Γ divides Ω into two disjoint regions: a simply connected interior region $\Omega^+ \Subset \Omega$ and an exterior annular region $\Omega^- = \Omega \setminus \Omega^+$. These satisfy the boundary conditions

$$\Gamma = \partial\Omega^+, \quad \partial\Omega^- = \Gamma \cup \partial\Omega. \quad (4.1)$$

The outer domain Ω and its boundary $\partial\Omega$ are fixed, while the internal curve Γ is an unknown to be determined as part of the optimization.

The curve Γ is parametrized by a smooth 2π -periodic function $f : \mathbb{S}^1 \rightarrow \mathbb{R}^2$, written as $x = f(\theta)$, where $\mathbb{S}^1$ denotes the unit circle, identified with $\mathbb{R}/2\pi\mathbb{Z}$. Thus, Γ is modeled as an immersion of the circle into the plane.

To ensure regularity, the parametrization f is assumed to satisfy the smoothness and non-degeneracy condition:

$$f \in C^r(\mathbb{S}^1), \quad r > 3, \quad 0 < c^{-1} < |\partial_\theta f(\theta)| < c. \quad (4.2)$$

This ensures that the curve is smooth, non-singular, and uniformly regular.

In addition, the chord-arc condition prevents self-intersections:

$$|f(\theta + \sigma) - f(\theta)| \geq c^{-1}|\sigma|, \quad \forall \theta \in \mathbb{R}, \quad \sigma \in [-\pi, \pi]. \quad (4.3)$$

From classical differential geometry, the arc length parameter s along the curve is defined by

$$s(\theta) = \int_0^\theta |\partial_\theta f(\theta')| d\theta', \quad (4.4)$$

and satisfies

$$ds = \sqrt{g} d\theta, \quad g = |\partial_\theta f|^2. \quad (4.5)$$

The derivative with respect to arc length is thus expressed as

$$\partial_s = \frac{1}{\sqrt{g}} \partial_\theta. \quad (4.6)$$

Assuming counterclockwise orientation, the unit tangent and normal vectors along the curve are defined as

$$\boldsymbol{\tau} = \partial_s f = \frac{1}{\sqrt{g}} \partial_\theta f, \quad \mathbf{n} = \boldsymbol{\tau}^\perp = (-\tau_2, \tau_1). \quad (4.7)$$

Here, $\boldsymbol{\tau}^\perp$ denotes a 90° counterclockwise rotation of the tangent vector. With this convention, the normal vector $\mathbf{n}$ points inward to Ω^+ and outward from Ω^- .

The curvature vector of the curve is given by

$$\mathbf{k} = \partial_s \boldsymbol{\tau} = \frac{1}{\sqrt{g}} \partial_\theta \left(\frac{\partial_\theta f}{\sqrt{g}} \right). \quad (4.8)$$

Its magnitude $|\mathbf{k}|$ is referred to as the scalar curvature.

To analyze deformations, the normal connection operator ∇_s is introduced. For any vector field f defined along the curve, it is given by

$$\nabla_s f = \partial_s f - \langle \boldsymbol{\tau}, \partial_s f \rangle \boldsymbol{\tau}, \quad (4.9)$$

which in two dimensions simplifies to

$$\nabla_s f = \langle \mathbf{n}, \partial_s f \rangle \mathbf{n}. \quad (4.10)$$

Finally, we adopt the following shorthand notations:

$$\partial_i = \partial_{x_i}, \quad i = 1, 2, \quad \partial = \partial_\theta. \quad (4.11)$$

These geometric tools form the foundation for analyzing curve evolution, deriving variational shape derivatives, and constructing gradient flow models in shape optimization.

4.3 Shape reconstruction from boundary measurements: an application in electrical impedance tomography

An important and illustrative application of shape optimization arises in the context of Electrical Impedance Tomography (EIT), a non-invasive imaging technique used

in fields such as medical diagnostics, geophysical exploration, and material science Pelletier and Vel, 2006. The objective of EIT is to determine the internal distribution of electrical conductivity within a domain by using boundary measurements of currents and voltages. In medical imaging, EIT is employed to detect abnormalities in biological tissues, whereas in geophysics it helps identify underground inclusions. A particularly relevant scenario occurs when the conductivity is assumed to be piecewise constant, in which case the problem reduces to identifying the shape and location of an unknown inclusion.

Let $\Omega \subset \mathbb{R}^2$ be a bounded, simply connected domain with smooth boundary $\partial\Omega$. Assume that the domain contains an unknown inclusion $\Omega^+ \Subset \Omega$, which is also simply connected and bounded by a smooth Jordan curve $\Gamma = \partial\Omega^+$. The remaining part of the domain is denoted by $\Omega^- := \Omega \setminus \overline{\Omega^+}$. The electric potential $u : \Omega \rightarrow \mathbb{R}$ satisfies the following transmission problem:

$$\begin{aligned} \operatorname{div}(a_0(x)\nabla u(x)) &= 0, \quad x \in \Omega, \\ \nabla u(x) \cdot v(x) &= q(x), \quad x \in \partial\Omega, \end{aligned} \tag{4.12}$$

where $v(x)$ denotes the unit outward normal vector on $\partial\Omega$, and $q \in L^2(\partial\Omega)$ is the prescribed Neumann boundary data. To ensure solvability, q is assumed to satisfy the standard compatibility condition:

$$\int_{\partial\Omega} q(x) \, ds(x) = 0. \tag{4.13}$$

The conductivity distribution $a_0(x)$ is defined piecewise by

$$a_0(x) = \begin{cases} a, & x \in \Omega^+, \\ 1, & x \in \Omega^-, \end{cases} \tag{4.14}$$

where $a > 0$ is a known constant different from 1. Under these conditions, the transmission problem admits a unique weak solution $u \in W^{1,2}(\Omega)$, which is additionally normalized to satisfy:

$$\int_{\partial\Omega} u(x) \, ds(x) = 0. \tag{4.15}$$

The inverse problem, known as the single measurement identification problem, can now be stated as follows: Given a target voltage distribution $P : \partial\Omega \rightarrow \mathbb{R}$ on the boundary, determine the inclusion Ω^+ such that the corresponding solution u to the Neumann problem satisfies the Dirichlet condition:

$$u(x) = P(x), \quad x \in \partial\Omega. \tag{4.16}$$

In other words, the goal is to reconstruct the shape of Ω^+ so that the resulting potential field matches the measured data on the boundary of the domain. This constitutes a nonlinear inverse problem, with several key challenges:

- **Nonlinearity:** The dependence of the solution u on the inclusion boundary Γ is highly nonlinear due to the discontinuity of the conductivity across Γ .
- **Ill-posedness:** Small perturbations in the data P may lead to large changes in the reconstructed shape. The problem may lack stability, uniqueness, or even solvability in the classical sense.
- **Instability:** Direct reconstruction is generally impractical. Regularization techniques and reformulation as optimization problems are typically required.

To address these difficulties, the problem is reformulated as a variational shape optimization problem. Let $\mathcal{O}$ denote the set of admissible shapes, typically represented by smooth Jordan curves $\Gamma \subset \Omega$. The objective is to find $\Gamma \in \mathcal{O}$ minimizing a suitable cost functional $\mathcal{J}(\Gamma)$, which measures the mismatch between computed and observed boundary data.

A widely used choice for $\mathcal{J}$ is the *Kohn–Vogelius functional*, defined by

$$\mathcal{J}_k(\Gamma) = \int_{\Omega} a_0(x) \nabla(u(x) - U(x)) \cdot \nabla(u(x) - U(x)) dx, \quad (4.17)$$

where:

- u is the solution to the Neumann problem:

$$\operatorname{div}(a_0 \nabla u) = 0 \quad \text{in } \Omega, \quad \nabla u \cdot \nu = q \quad \text{on } \partial\Omega, \quad (4.18)$$

- U is the solution to the Dirichlet problem:

$$\operatorname{div}(a_0 \nabla U) = 0 \quad \text{in } \Omega, \quad U = P \quad \text{on } \partial\Omega. \quad (4.19)$$

The solutions of elliptic problems in Ω are understood in a weak sense in the Sobolev space $H^1(\Omega)$, and the equations are written in $\mathcal{D}'(\Omega)$ in the sense of distributions.

The Kohn–Vogelius functional evaluates the discrepancy between the solutions to the Neumann and Dirichlet problems. It vanishes if and only if $u = U$ in Ω , indicating a perfect match and, hence, a correct reconstruction of the inclusion shape.

The forward mapping $\Gamma \mapsto u$ defines a nonlinear operator from the set of admissible shapes $\mathcal{O}$ into the Sobolev space $W^{1,2}(\Omega)$. Consequently, minimizing $\mathcal{J}_k(\Gamma)$

yields a nonlinear and PDEs constrained shape optimization problem. Analytical and numerical treatment of this problem typically involves tools such as shape differentiation, sensitivity analysis, and gradient-based optimization algorithms, including both geometric flows and topological derivative methods.

4.4 Regularization and geometric control in shape optimization

In shape optimization problems, particularly those involving inverse identification such as Electrical Impedance Tomography Cahn and Hilliard, 1958, solutions may fail to exist or be unstable when geometric constraints are absent. This ill-posedness typically results from the lack of compactness in the admissible set of shapes. Minimizing sequences may converge to degenerate configurations, such as shapes with fine-scale oscillations or fractal-like boundaries, rather than to smooth geometric domains. To overcome these issues and ensure the well-posedness of the optimization problem, it is standard practice to incorporate geometric regularization into the cost functional.

In free boundary problems, the interface of the inclusion domain Ω^+ is described by a Jordan curve $\Gamma \subset \Omega$. To stabilize the optimization process and control the geometric properties of Γ , regularization terms are added to the objective functional. Each term serves a specific role in penalizing undesirable geometric features.

The most basic and widely used regularization is the perimeter energy, which measures the total length of the curve and discourages excessively large or complex boundaries. It is given by

$$\mathcal{E}_p(\Gamma) = \int_{\Gamma} ds = \int_0^{2\pi} \sqrt{g(\theta)} d\theta, \quad (4.20)$$

where $g(\theta) = |\partial_{\theta} f(\theta)|^2$ denotes the squared norm of the derivative of the parameterization $f : \mathbb{S}^1 \rightarrow \mathbb{R}^2$. The perimeter energy has analogies with the Mumford–Shah functional in image segmentation and, from a physical perspective, represents capillary or surface tension energy. Mathematically, bounded perimeter energy ensures that the curve remains of controlled size, though it may still develop corners or nonsmooth segments.

To promote higher regularity and suppress oscillatory features, the Euler elastica energy (also known as the one-dimensional Willmore energy) is often employed:

$$\mathcal{E}_e(\Gamma) = \frac{1}{2} \int_{\Gamma} |\mathbf{k}|^2 ds, \quad (4.21)$$

where $|\mathbf{k}|$ denotes the curvature magnitude along the curve. This energy penalizes bending and favors smooth, gently curved boundaries. It has proven effective in both geometric optimization and image processing applications.

From a functional-analytic viewpoint, the simultaneous finiteness of $\mathcal{E}_p(\Gamma)$ and $\mathcal{E}_e(\Gamma)$ implies that the natural arc-length parameterization $f(s)$ of Γ belongs to the Hölder space $C^{1+\kappa}(\mathbb{S}^1)$ for some $0 \leq \kappa < \frac{1}{2}$. This guarantees that the curve has continuous tangents and avoids pathological behavior, with both diameter and curvature remaining under control.

In practical applications, such as the minimization of the Kohn–Vogelius functional $\mathcal{J}_k$ discussed in the previous section, it is customary to combine the objective with geometric regularization. The resulting total functional takes the form:

$$\mathcal{J}_{\text{reg}}[f] = \varepsilon_e \mathcal{E}_e[f] + \varepsilon_p \mathcal{E}_p[f] + \mathcal{J}_\alpha[f], \quad (4.22)$$

where $\varepsilon_e, \varepsilon_p > 0$ are small regularization parameters that balance fidelity to the physical model (via $\mathcal{J}_\alpha$) with control over boundary complexity and smoothness. Here, α may denote a specific modeling context, such as k for Kohn–Vogelius or b for Bernoulli-type objectives.

An important modeling consideration is whether to define these functionals on geometric curves $\Gamma \subset \mathbb{R}^2$ or on their parameterizations, i.e., smooth immersions $f : \mathbb{S}^1 \rightarrow \mathbb{R}^2$ satisfying the non-degeneracy condition $|\partial_\theta f| > 0$. Although the functionals $\mathcal{E}_p$, $\mathcal{E}_e$, and $\mathcal{J}_\alpha$ are invariant under reparameterization and depend only on the geometric shape $\Gamma = f(\mathbb{S}^1)$, there are compelling theoretical and practical reasons to work in the space of immersions:

- *Numerical Discretization:* Approximating a geometric curve directly requires moving mesh methods, which are complex and computationally intensive. In contrast, parameterizing the curve as a periodic function $f(\theta)$ allows the use of well-established tools such as Fourier series or spline interpolation, enabling efficient and robust numerical schemes.
- *Gradient Flow Formulation:* Many shape optimization methods are implemented via gradient flows of the objective functional. These flows are naturally defined in the space of mappings rather than in the space of geometric shapes, and they are generally not invariant under reparameterization. Therefore, treating f as the optimization variable is essential for rigorous gradient flow analysis and numerical evolution.

As a result, all functionals involved in the shape optimization process are considered as functionals of the immersion f , denoted $\mathcal{E}_\beta[f]$ and $\mathcal{J}_\alpha[f]$, where $f \in C^2(\mathbb{S}^1, \mathbb{R}^2)$ is assumed to be a regular, non-degenerate immersion.

4.5 Shape derivatives and gradient flow evolution

In shape optimization, the control variable is not a scalar or vector-valued function, but rather a geometric entity—such as a boundary curve or a subdomain—whose deformation influences the value of a cost functional. This distinguishes shape optimization from classical variational problems and necessitates the development of a dedicated analytical toolset known as *shape calculus*. The main goal of shape calculus is to compute the first- and second-order variations of functionals with respect to domain deformations, enabling sensitivity analysis and the application of gradient-based optimization algorithms.

Let $\Gamma = f(\mathbb{S}^1)$ be a smooth, closed curve in $\mathbb{R}^2$, defined by a regular immersion $f : \mathbb{S}^1 \rightarrow \mathbb{R}^2$. Suppose a shape-dependent functional $\mathcal{E}[f]$ is invariant under reparameterization, meaning it depends solely on the geometry of Γ . Given a smooth vector field δf defined on $\mathbb{S}^1$, representing an infinitesimal perturbation of the curve, the first variation (Gâteaux derivative) of $\mathcal{E}$ is defined by

$$\mathcal{E}'[f]\delta f := \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} (\mathcal{E}[f + \varepsilon \delta f] - \mathcal{E}[f]). \quad (4.23)$$

Under geometric invariance, the Hadamard structure theorem ensures that this derivative can be expressed as

$$\mathcal{E}'[f]\delta f = \int_{\Gamma} \mathcal{A}[f] \langle \delta f, \mathbf{n} \rangle ds, \quad (4.24)$$

where $\mathbf{n}$ is the unit normal vector to the curve and $\mathcal{A}[f]$ is a scalar function defined on Γ . This shows that the shape derivative depends only on the normal component of the deformation. The corresponding shape gradient (also called the Hadamard gradient) is then given by

$$\mathcal{A} := \mathcal{A}[f]\mathbf{n}, \quad (4.25)$$

which defines a vector field on the curve pointing in the steepest ascent direction of the functional.

We now illustrate this framework by computing the Hadamard gradients of the regularization terms introduced earlier.

The *perimeter energy* is defined as

$$\mathcal{E}_p[f] = \int_{\Gamma} ds = \int_0^{2\pi} \sqrt{g(\theta)} d\theta, \quad (4.26)$$

and its shape gradient is given by

$$\mathcal{A}_p = -\mathbf{k}, \quad (4.27)$$

where $\mathbf{k}$ is the curvature vector of the curve.

The *elastica energy*, or bending energy, is defined as

$$\mathcal{E}_e[f] = \frac{1}{2} \int_{\Gamma} |\mathbf{k}|^2 ds, \quad (4.28)$$

and its shape gradient takes the form

$$\mathcal{A}_e = \nabla_s \nabla_s \mathbf{k} + \frac{1}{2} |\mathbf{k}|^2 \mathbf{k}, \quad (4.29)$$

where ∇_s is the normal projection of the arc-length derivative, i.e., the covariant derivative along the curve.

In many inverse problems, the objective functional involves the solution to PDEs defined on the domain. A typical example is the Kohn–Vogelius functional, which compares solutions of Neumann and Dirichlet boundary value problems. The associated shape gradient is given by

$$\mathcal{B}_k = 2 (a_0 \partial_n u [\partial_n u] - a_0 \partial_n U [\partial_n U]) \mathbf{n} - [a_0 |\nabla u|^2 - a_0 |\nabla U|^2] \mathbf{n}, \quad (4.30)$$

where u and U are the solutions to the Neumann and Dirichlet problems, respectively, and $[\cdot]$ denotes the jump across the interface Γ . An important feature of this expression is that it depends only on the state variables, not on their shape derivatives—this makes the Kohn–Vogelius functional particularly suitable for numerical optimization.

Having determined the shape gradients of the objective and regularization terms, one can define a geometric evolution equation describing the descent of the shape along the steepest descent direction. Specifically, for the regularized cost functional

$$\mathcal{J}_{\text{reg}}[f] = \varepsilon_e \mathcal{E}_e[f] + \varepsilon_p \mathcal{E}_p[f] + \mathcal{J}_k[f], \quad (4.31)$$

the gradient flow is given by

$$\partial_t f + \mathcal{A}[f] + \mathcal{B}_k[f] = 0, \quad f|_{t=0} = f_0, \quad (4.32)$$

where

$$\mathcal{A}[f] = \varepsilon_e \mathcal{A}_e[f] + \varepsilon_p \mathcal{A}_p[f] \quad (4.33)$$

is the total regularization gradient, and $\mathcal{B}_k[f]$ is the shape gradient of the Kohn–Vogelius term. This flow defines a curve evolution equation in the space of immersions, ensuring monotonic decrease of the objective and driving the curve toward an optimal configuration.

As a special case, if only geometric regularization is considered (i.e., without PDE-dependent terms), the flow reduces to a purely geometric evolution:

$$\partial_t f + \mathcal{A}_e[f] + \mathcal{A}_p[f] = 0, \quad (4.34)$$

which is a combination of curvature-driven flows: the elastica (or Willmore-type) flow and the curve shortening flow. These models are widely studied in geometric analysis and appear in applications such as contour smoothing, filament modeling, and interface dynamics in materials science.

4.6 Representation of shape gradients in fixed function spaces

In the analysis and computation of shape optimization problems, the Gâteaux derivative (also known as the variational derivative) plays a central role in characterizing how a functional responds to infinitesimal variations in the shape. As discussed earlier, for functionals defined on immersed curves $f : \mathbb{S}^1 \rightarrow \mathbb{R}^2$, the first-order shape derivative—also called the Hadamard derivative—takes the general form

$$\mathcal{E}'[f]\delta f = \int_{\Gamma} \mathcal{A}[f] \langle \delta f, \mathbf{n} \rangle ds, \quad (4.35)$$

where $\mathcal{A}[f]$ is a scalar function defined along the curve $\Gamma = f(\mathbb{S}^1)$, $\mathbf{n}$ is the unit normal vector, and ds is the arc length element. The perturbation δf is an arbitrary smooth vector field on $\mathbb{S}^1$, representing an infinitesimal deformation of the curve.

This representation reveals two key structural features:

- The derivative $\mathcal{E}'[f]$ acts linearly on the deformation δf , making it a continuous linear functional.
- The variation depends only on the *normal component* of δf , i.e., $\langle \delta f, \mathbf{n} \rangle$, reflecting the geometric nature of shape deformations.

By the Riesz representation theorem, any continuous linear functional on a Hilbert space can be identified with an inner product against a unique element of that space. Thus, if we view δf as an element of $L^2(\Gamma)$, the Hadamard gradient defines a natural geometric gradient in this space.

However, this leads to a subtle but significant difficulty: the Hilbert space $L^2(\Gamma, ds)$ depends on the current shape, because the arc length measure ds is defined through the immersion f . More precisely, $ds = \sqrt{g(\theta)} d\theta$, where $g(\theta) = |\partial_\theta f(\theta)|^2$ is the squared local stretch of the parameterization. Therefore, the shape gradient lives in a *shape-dependent function space*, which varies with f .

This shape-dependence introduces analytical and computational challenges:

- The function space $L^2(\Gamma)$ changes as the shape evolves, making it difficult to define gradients, Hessians, and evolution flows in a consistent framework.
- The shape gradient cannot be interpreted as a Fréchet derivative in a fixed Hilbert space, which complicates the development of higher-order optimization methods.
- Numerical implementations relying on discretizations over $\mathbb{S}^1$ must reconcile the mismatch between the geometric domain Γ and the computational parameter domain.

To resolve these issues, it is advantageous to recast all computations in a fixed function space—namely, the space $L^2(\mathbb{S}^1)$ of square-integrable functions on the parameter domain. This approach is consistent with the immersion-based formulation adopted throughout the analysis, and it offers several important benefits:

- It allows gradient flows and optimization algorithms to be defined in a fixed Hilbert space, avoiding the complications of variable integration domains.
- It provides a unified setting for deriving second-order variations, adjoint equations, and implementing numerical schemes such as spectral or finite-difference discretizations.

To convert the Hadamard gradient into this fixed space, we observe that the arc length measure satisfies $ds = \sqrt{g(\theta)} d\theta$.

This reformulation identifies $\sqrt{g(\theta)} \mathcal{A}[f](\theta)$ as the natural representative of the gradient in the Hilbert space $L^2(\mathbb{S}^1)$. That is, the gradient of the functional $\mathcal{E}[f]$ can be written in the form

$$\mathcal{A}(\theta) = \sqrt{g(\theta)} \mathcal{A}[f](\theta) \mathbf{n}(\theta), \quad (4.36)$$

which belongs to $L^2(\mathbb{S}^1; \mathbb{R}^2)$ and is independent of the geometric length element. This expression retains the geometric interpretation of the Hadamard gradient—namely, that descent occurs in the normal direction—while making it compatible with fixed-domain function spaces. This facilitates the development of well-posed gradient flow equations, variational formulations, and numerical implementations.

By recasting the entire optimization framework into the fixed parameter space $\mathbb{S}^1$, we achieve a balance between geometric fidelity and analytical tractability. This reformulation paves the way for the design of stable numerical algorithms, such as curvature-driven flows, Newton-type iterations, or preconditioned gradient descent, all of which operate within a consistent functional setting.

4.7 Second-order shape derivatives and hessian structure of Kohn-Vogelius functionals

The Kohn–Vogelius functional represents a central class of objective functionals in shape optimization. It measures the discrepancy between two solutions to boundary value problems—typically with Dirichlet and Neumann boundary conditions—and arises naturally in applications such as electrical impedance tomography (EIT), material detection, and free boundary problems.

In the previous sections, we introduced the Hadamard gradient and demonstrated how its reparameterization-invariant form can be recast into a fixed Hilbert space such as $L^2(\mathbb{S}^1)$ for both theoretical consistency and numerical implementation. To further analyze the local structure of the optimization problem—particularly for assessing convergence and stability of gradient flows—we now investigate the second-order variation, or shape Hessian, of such functionals.

Linearized Flow and Moving Frame Decomposition. We consider the linearization of the gradient flow around a given shape. Let δf denote a small perturbation of the immersion f , and assume that the evolution of this perturbation satisfies the linearized system

$$\partial_t \delta f + \mathcal{R}'[f] \delta f + \mathcal{B}'_\alpha[f] \delta f = \mathbf{F}, \quad \delta f|_{t=0} = 0, \quad (4.37)$$

where $\mathcal{R}'[f]$ and $\mathcal{B}'_\alpha[f]$ are the Gâteaux derivatives of the regularization and main objective terms, and $\mathbf{F}$ is an external forcing.

To express the perturbation in geometric terms, we decompose it along the natural

frame of the curve:

$$\delta f = \omega \mathbf{n} + \varsigma \boldsymbol{\tau}, \quad (4.38)$$

where ω and ς are scalar functions on $\mathbb{S}^1$ representing the normal and tangential components of the variation, and $\mathbf{n}, \boldsymbol{\tau}$ are the unit normal and tangent vectors to the curve.

Let us assume the Hadamard gradient of the functional is of the form $\mathcal{A}[f] = \mathcal{A}[f] \mathbf{n}$, where $\mathcal{A}[f]$ is a scalar field on Γ . Then the Gâteaux derivative $\mathcal{A}'[f]\delta f$ can be expanded using the moving frame decomposition as

$$\mathcal{A}'[f]\delta f = (\mathbf{A}_{11}\omega + \mathbf{A}_{12}\varsigma) \mathbf{n} + (\mathbf{A}_{21}\omega + \mathbf{A}_{22}\varsigma) \boldsymbol{\tau}. \quad (4.39)$$

In matrix form, this becomes:

$$\mathcal{A}'[f]\delta f = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \omega \\ \varsigma \end{pmatrix}. \quad (4.40)$$

To compute the components $\mathbf{A}_{ij}$, we use the assumption that $\mathcal{A}[f]$ is invariant under reparameterization. For any smooth diffeomorphism $\phi : \mathbb{S}^1 \rightarrow \mathbb{S}^1$, this implies

$$\mathcal{A}[f \circ \phi] = \mathcal{A}[f] \circ \phi. \quad (4.41)$$

Under this condition, the variations in $\mathcal{A}[f]$ along the tangential and normal directions yield:

$$\begin{aligned} \mathbf{A}_{12}[f]\varsigma &= \frac{1}{\sqrt{g}} \partial_\theta \mathcal{A}[f] \cdot \varsigma, \\ \mathbf{A}_{21}[f]\omega &= -\frac{1}{\sqrt{g}} \mathcal{A}[f] \cdot \partial_\theta \omega, \end{aligned} \quad (4.42)$$

$$\begin{aligned} \mathbf{A}_{22}[f]\varsigma &= -K\varsigma, \\ \mathbf{A}_{11}[f]\omega &= \mathcal{A}[f] \cdot \omega, \end{aligned}$$

where $g = |\partial_\theta f|^2$ is the metric factor and K denotes the curvature scalar. However, the resulting operator matrix is generally not symmetric, which limits its direct use in Newton-type methods or stability analysis.

Symmetrization in Fixed Function Space

To address this issue, we move to the fixed Hilbert space $L^2(\mathbb{S}^1)$ and define the L^2 -gradient of the functional as

$$\nabla_{L^2} \mathcal{E}[f] := \sqrt{g} \cdot \mathcal{A}[f]. \quad (4.43)$$

Using the product rule, the corresponding Gâteaux derivative becomes

$$(\sqrt{g}\mathcal{A})'[f]\delta f = \sqrt{g}\mathcal{A}'[f]\delta f + (\sqrt{g})'[f] \cdot \mathcal{A}[f], \quad (4.44)$$

with the variation of $\sqrt{g}$ computed as

$$(\sqrt{g})'[f]\delta f = -\sqrt{g}K\omega + \partial_\theta\varsigma. \quad (4.45)$$

Substituting these into the linearized system gives the symmetric form of the L^2 -Hessian:

$$(\sqrt{g}\mathcal{A})'[f]\delta f = \begin{pmatrix} \sqrt{g}\mathbf{A}_{11} - \sqrt{g}K\mathcal{A} & \frac{1}{\sqrt{g}}\partial_\theta(\mathcal{A}\cdot) \\ -\mathcal{A} \cdot \partial_\theta & -\sqrt{g}K \end{pmatrix} \begin{pmatrix} \omega \\ \varsigma \end{pmatrix}. \quad (4.46)$$

This operator is self-adjoint in the $L^2(\mathbb{S}^1)$ inner product and provides a rigorous basis for:

- local stability analysis of shape evolution flows;
- convergence studies for Newton-type or preconditioned gradient algorithms;
- spectral analysis of optimal shapes and regularity properties.

By lifting the Hessian formulation into the fixed space $L^2(\mathbb{S}^1)$, we maintain geometric accuracy while achieving analytical and numerical robustness. This completes the transition from first-order to second-order shape analysis in a fully variational and geometrically consistent framework.

4.7.1 Second-order structure and local well-posedness of gradient flow evolution

This section focuses on the derivation and analysis of the second-order shape derivatives—i.e., Hessians—of the energy functionals $\mathcal{T}_\alpha$ and $\mathcal{E}_\beta$. These functionals correspond respectively to interface-type and geometric-type energies. Their Gâteaux derivatives provide essential tools for higher-order optimization, sensitivity analysis, and theoretical stability results.

Both $\mathcal{T}_\alpha$ and $\mathcal{E}_\beta$ possess the required structural regularity and variational properties for second-order shape derivative analysis. In particular, their Hadamard gradients admit well-defined Gâteaux derivatives $\mathcal{B}'_\alpha$ and $\mathcal{A}'_\beta$, which take the form of matrix-valued operators acting on the shape variation vector $\delta f = \omega\mathbf{n} + \varsigma\boldsymbol{\tau}$, with ω and ς denoting the normal and tangential components.

These derivatives can be expressed in the structured matrix form:

$$\mathcal{B}'_\alpha[f]\delta f = \begin{pmatrix} \mathbf{B}_{11}^\alpha & \frac{1}{\sqrt{g}}\partial_\theta\mathcal{B}_\alpha \\ -\frac{1}{\sqrt{g}}\mathcal{B}_\alpha\partial_\theta & -K \end{pmatrix} \begin{pmatrix} \omega \\ \varsigma \end{pmatrix}, \quad \mathcal{A}'_\beta[f]\delta f = \begin{pmatrix} \mathbf{A}_{11}^\beta & \frac{1}{\sqrt{g}}\partial_\theta\mathcal{A}_\beta \\ -\frac{1}{\sqrt{g}}\mathcal{A}_\beta\partial_\theta & -K \end{pmatrix} \begin{pmatrix} \omega \\ \varsigma \end{pmatrix}. \quad (4.47)$$

Here, $\mathcal{A}_\beta = \mathbf{A}_\beta \cdot \mathbf{n}$ and $\mathcal{B}_\alpha = \mathbf{B}_\alpha \cdot \mathbf{n}$ are the scalar projections of the Hadamard gradients onto the normal direction, $g = |\partial_\theta f|^2$ is the local metric factor, and K is the curvature. This matrix structure reveals the inherent coupling between normal and tangential perturbations in second-order shape responses.

Examples: Hessians of Geometric Energies.

For geometric regularization energies, such as the capillary energy $\mathcal{E}_p$ and the elastic (bending) energy $\mathcal{E}_e$, the leading-order Hessians take the form of quasi-linear differential operators:

$$\begin{aligned} A_{11}^e \omega &= \partial_s^4 \omega + \frac{5}{2} K \partial_s (K \partial_s \omega) + (3K \mathcal{A}_e + 3(\partial_s K)^2 + K \partial_s^2 K) \omega, \\ A_{11}^p \omega &= -\partial_s^2 \omega - K^2 \omega, \end{aligned} \quad (4.48)$$

where ∂_s is the arc-length derivative. These expressions demonstrate the strong dependence of the second-order variation on curvature and its derivatives, reflecting the geometric sensitivity of the energy functionals.

To simplify analysis, we separate out a class of lower-order smoothing terms represented by a bounded operator $\mathbf{R}$. For $\omega \in H_\sharp^0$ and $f \in H_\sharp^{r+s}$, we have the estimate:

$$\|\mathbf{R}\omega\|_{H_\sharp^s} \leq c(r, s) \left(1 + \|f\|_{H_\sharp^{r+s}}\right) \|\omega\|_{H_\sharp^0}, \quad (4.49)$$

showing that these remainders do not affect the leading spectral behavior of the Hessian.

Transmission-Based Energies and Holomorphic Representation.

For interface-type functionals such as $\mathcal{T}_\alpha$ —notably the Kohn–Vogelius functional—we rely on harmonic transmission problems between subdomains Ω^+ and Ω^- to define state functions u and U . These functions satisfy transmission conditions across $\Gamma = \partial\Omega^+$ and boundary conditions on $\partial\Omega$. Their harmonic conjugates v and V allow us to represent the state solutions as complex-valued functions $w = u + iv$, $W = U + iV$, which are holomorphic in each subdomain.

Using this holomorphic structure, we derive the second-order Hadamard variation in terms of boundary-integral representations. Specifically, the operator $\mathbf{B}_{11}^k[f]$ —

appearing in the Hessian of the Kohn–Vogelius functional—has the form:

$$\mathbf{B}_{11}^k[f]\omega = \frac{\lambda}{\sqrt{g}}(\mathbf{A}_N - \mathbf{A}_D)\omega + \mathbf{c} \cdot \omega + \mathbf{R}[f]\omega, \quad (4.50)$$

where:

- $\lambda = \frac{2(a-1)^2}{a+1}$ is a contrast-dependent constant;
- $\mathbf{A}_N, \mathbf{A}_D$ are symmetric pseudodifferential operators given by:

$$\begin{aligned} \mathbf{A}_N\omega &= a \partial_s v^+ \cdot |\partial_\theta|(\partial_s v^+\omega) - \partial_s u^+ \cdot |\partial_\theta|(\partial_s u^+\omega), \\ \mathbf{A}_D\omega &= a \partial_s V^+ \cdot |\partial_\theta|(\partial_s V^+\omega) - \partial_s U^+ \cdot |\partial_\theta|(\partial_s U^+\omega); \end{aligned} \quad (4.51)$$

- $\mathbf{c}$ is a smooth coefficient given by:

$$\mathbf{c} = \frac{4a(a-1)}{a+1} [\partial_s u^+ \cdot \partial_s^2 v^+ - \partial_s v^+ \cdot \partial_s^2 u^+ - (\partial_s U^+ \cdot \partial_s^2 V^+ - \partial_s V^+ \cdot \partial_s^2 U^+)] + 2\mathcal{B}_k K. \quad (4.52)$$

This formulation reveals the subtle balance between physical contrast, curvature, and harmonic structure of the state fields.

Well-Posedness via Nash–Moser Theory.

To conclude, we return to the full gradient flow system:

$$\partial_t f + \mathcal{M}[f] + \mathcal{B}_\alpha[f] = 0, \quad f(0) = f_0, \quad (4.53)$$

where $\mathcal{M}[f]$ denotes the total regularization term:

$$\mathcal{M}[f] = \varepsilon_e \mathcal{A}_e + \varepsilon_m \mathcal{A}_m + \varepsilon_p \mathcal{A}_p, \quad (4.54)$$

with regularization weights $\varepsilon_e > 0$ and $\varepsilon_m, \varepsilon_p \geq 0$.

Two main analytical difficulties arise:

- The system is not parabolic—it lacks smoothing properties, making standard theory inapplicable;
- Transitioning to the moving frame introduces derivative loss, resulting in failure of convergence in naive Newton schemes.

To resolve these issues, we employ the Nash–Moser implicit function theorem, which is specifically designed for ill-posed problems with derivative loss. It provides a robust framework for proving local existence under high-regularity assumptions and mild smoothing.

Existence Theorem (Nash–Moser). Let $\mathbb{X}^r$ denote the Hilbert space of immersions $f : \mathbb{S}^1 \times (0, T) \rightarrow \mathbb{R}^2$ satisfying:

$$\|f\|_r^2 = \|f(\cdot, 0)\|_{H_\#^r}^2 + \int_0^T \|f(\cdot, t)\|_{H_\#^r}^2 dt. \quad (4.55)$$

Then the following holds:

Theorem 4.7.1. *Let $f_0 \in H_\#^{r+\lambda}$ be a regular initial immersion with $r \geq 1$ and $\lambda = 42r$, satisfying Condition 1.2.1. Then for every $\eta > 0$, there exists $T > 0$ and a solution $f(t)$ to the gradient flow equation such that:*

$$\|f(t) - f_0\|_{H_\#^r} \leq c_\lambda \eta, \quad (4.56)$$

where c_λ depends only on $\|f_0\|_{H_\#^{r+\lambda}}$.

Proof. This theorem is borrowed from the forthcoming book by P.I. Plotnikov and J. Sokolowski to appear in SpringerBriefs on PDEs and Data Science, where the complete proof is given. $\square$

Although the regularity assumptions in this theorem are far from optimal, they suffice for demonstrating local solvability using the classical Nash–Moser scheme. Improved versions with sharper constants and weaker smoothness requirements can be obtained using more advanced techniques, which are beyond the scope of this exposition.

4.8 Interface optimization in two-phase transmission problems

We consider a prototypical two-phase interface problem governed by an elliptic transmission system, where the geometry of an internal interface Γ is to be optimized to minimize the mismatch between solutions corresponding to different boundary conditions. Such problems arise naturally in composite material design, inverse conductivity identification (e.g., EIT), and free boundary problems.

Let $\Omega \subset \mathbb{R}^2$ be a bounded smooth domain, partitioned by an unknown closed curve Γ into two subdomains: an interior region $\Omega^+ \Subset \Omega$ and an exterior annulus $\Omega^- := \Omega \setminus \overline{\Omega^+}$. In each subdomain, the state variable u satisfies the Poisson equation with a piecewise constant diffusion coefficient $a(x)$:

$$\begin{cases} -\nabla \cdot (a_1 \nabla u_1) = 0 & \text{in } \Omega^+, \\ -\nabla \cdot (a_2 \nabla u_2) = 0 & \text{in } \Omega^-, \\ u_1 = u_2, \quad a_1 \nabla u_1 \cdot \mathbf{n} = a_2 \nabla u_2 \cdot \mathbf{n} & \text{on } \Gamma, \\ u_1 = 0 & \text{on } \Gamma_i, \\ a_2 \nabla u_2 \cdot \mathbf{n} = F, \quad u_2 = G & \text{on } \Gamma_e. \end{cases} \quad (4.57)$$

Here, Γ_i and Γ_e denote complementary subsets of $\partial\Omega$, and $\mathbf{n}$ is the unit normal vector pointing from Ω^- to Ω^+ . The boundary data F (Neumann) and G (Dirichlet) are assumed given.

To quantify the difference in state behavior under these two boundary scenarios, we introduce the Kohn–Vogelius functional:

$$J(\Gamma) := \int_{\Omega} a(x) |\nabla(w - v)|^2 dx. \quad (4.58)$$

The auxiliary problems for w and v are:

$$\begin{cases} -\nabla \cdot (a \nabla w) = 0 & \text{in } \Omega = \Omega^+ \cup \Omega^-, \\ [w] = 0, \quad [a \nabla w \cdot \mathbf{n}] = 0 & \text{on } \Gamma, \\ w = 0 & \text{on } \Gamma_i, \\ w = G & \text{on } \Gamma_e, \end{cases} \quad (4.59)$$

$$\begin{cases} -\nabla \cdot (a \nabla v) = 0 & \text{in } \Omega = \Omega^+ \cup \Omega^-, \\ [v] = 0, \quad [a \nabla v \cdot \mathbf{n}] = 0 & \text{on } \Gamma, \\ v = 0 & \text{on } \Gamma_i, \\ a(x) \nabla v \cdot \mathbf{n} = F & \text{on } \Gamma_e. \end{cases} \quad (4.60)$$

The shape derivative of J with respect to a normal deformation of the interface is:

$$dJ = [2a(\partial_n v [\partial_n v] - \partial_n w [\partial_n w]) - a(|\nabla v|^2 - |\nabla w|^2)] \mathbf{n}. \quad (4.61)$$

Geometric Framework and Gradient Flow

We parameterize the interface Γ via a smooth closed curve $f : \mathbb{S}^1 \rightarrow \mathbb{R}^2$ with arc-length element:

$$ds = \sqrt{g(\theta)} d\theta, \quad g(\theta) = |\partial_\theta f|^2. \quad (4.62)$$

The tangent, normal, and curvature vectors are:

$$\boldsymbol{\tau} = \partial_s f, \quad \mathbf{n} = \boldsymbol{\tau}^\perp, \quad \mathbf{k} = \partial_s^2 f. \quad (4.63)$$

The normal projection of a derivative is:

$$\nabla_s \Phi = \partial_s \Phi - (\partial_s \Phi \cdot \boldsymbol{\tau}) \boldsymbol{\tau}. \quad (4.64)$$

We define two geometric regularization energies:

$$\mathcal{L} = \int_\Gamma ds, \quad \mathcal{E}_e = \frac{1}{2} \int_\Gamma |\mathbf{k}|^2 ds. \quad (4.65)$$

Their shape derivatives are:

$$d\mathcal{L}(f) = -\mathbf{k}, \quad d\mathcal{E}_e(f) = \nabla_s \nabla_s \mathbf{k} + \frac{1}{2} |\mathbf{k}|^2 \mathbf{k}. \quad (4.66)$$

Combining with dJ , the total shape gradient is:

$$d\mathcal{J}(f) = d\mathcal{E}_e(f) + d\mathcal{L}(f) + dJ(f). \quad (4.67)$$

The corresponding geometric gradient flow equation is:

$$\partial_t f + \varepsilon (\nabla_s \nabla_s \mathbf{k} + \frac{1}{2} |\mathbf{k}|^2 \mathbf{k} - \mathbf{k}) + dJ = 0, \quad f(0) = f_0. \quad (4.68)$$

In the special case $dJ = 0$, the flow reduces to the Willmore flow:

$$\partial_t f + \nabla_s \nabla_s \mathbf{k} + \frac{1}{2} |\mathbf{k}|^2 \mathbf{k} - \mathbf{k} = 0. \quad (4.69)$$

4.8.1 Numerical examples

Example 4.8.1. Consider the annular domain $\Omega = B(0, r_2) \setminus B(0, r_1)$, where $0 < r_1 < r_2$. Inside Ω , the unknown interface is given by a moving radius $R(t)$ satisfying $r_1 < R(t) < r_2$. This interface divides Ω into two subdomains:

- The interior region $\Omega^+ = B(0, R(t)) \setminus B(0, r_1)$;
- The exterior region $\Omega^- = B(0, r_2) \setminus B(0, R(t))$.

The piecewise constant diffusion coefficient $a(x)$ is defined as:

$$a(x) = \begin{cases} 2.0 & \text{if } x \in \Omega^+, \\ 1.0 & \text{if } x \in \Omega^-. \end{cases} \quad (4.70)$$

The Kohn–Vogelius functional becomes:

$$J(R) = \int_{\Omega} a(x) |\nabla w_R - \nabla v_R|^2 dx. \quad (4.71)$$

The state equations are:

$$\begin{cases} -\nabla \cdot (a \nabla w) = 0 & \text{in } \Omega, \\ w = G & \text{on } \partial\Omega, \\ w = 0 & \text{on } \Gamma, \end{cases} \quad (4.72)$$

$$\begin{cases} -\nabla \cdot (a \nabla v) = 0 & \text{in } \Omega, \\ a \frac{\partial v}{\partial n} = F & \text{on } \partial\Omega, \\ v = 0 & \text{on } \Gamma. \end{cases} \quad (4.73)$$

Due to radial symmetry, w and v can be solved explicitly. Choosing $G \approx 2.5902671654$ and $F = 1.0$ ensures that the true radius $R^* = 1.0$ yields $J(R^*) = 0$.

We evolve the radius via:

$$\partial_t f + \varepsilon (\nabla_s \nabla_s \mathbf{k} + \frac{1}{2} |\mathbf{k}|^2 \mathbf{k} - \mathbf{k}) + dJ = 0, \quad f(0) = f_0. \quad (4.74)$$

Using RK4 with time step $h = 0.01$, $R(0) \in \{0.5, 1.5\}$, and $\varepsilon \in \{0, 0.1, 0.5, 1.0, 2.0\}$, the interface radius converges toward R^* , validating the shape optimization model. To visualize the impact of regularization, we compare several runs with different values of $\varepsilon \in \{0, 0.1, 0.5, 1.0, 2.0\}$. The evolution of the interface radius $R(t)$ under different regularization strengths is depicted in Figures 4.1, 4.2, 4.3, 4.4, and 4.5, corresponding to increasing values of ε . These results clearly demonstrate that stronger regularization promotes smoother and more stable convergence toward the true interface radius $R^* = 1.0$.

Example 4.8.2. We consider a two-phase free boundary identification problem, where the goal is to reconstruct the geometry of the internal interface $\Gamma = \partial\Omega^+$ by minimizing a mismatch functional based on solutions to elliptic transmission problems. The domain is the annulus $\Omega = B(0, r_{\text{outer}}) \setminus B(0, r_{\text{inner}})$, with $r_{\text{inner}} = 0.3$ and $r_{\text{outer}} = 2.0$. The

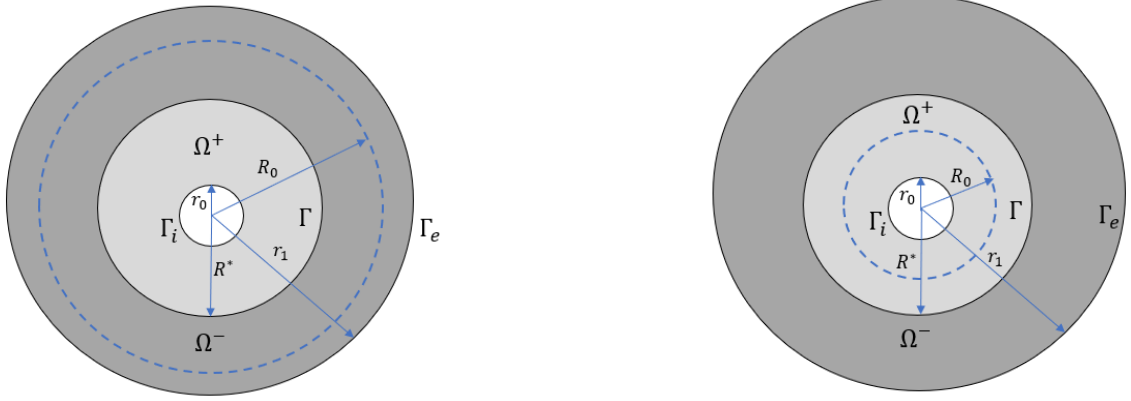


Figure 4.1: Initial Interface diagram (Two initial conditions are considered: $R_0 = 1.5$ and $R_0 = 0.5$.)

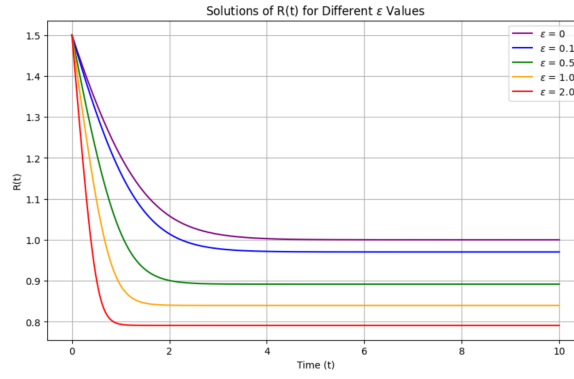


Figure 4.2: Evolution of $R(t)$ with $R_0 = 1.5$ for various ε .

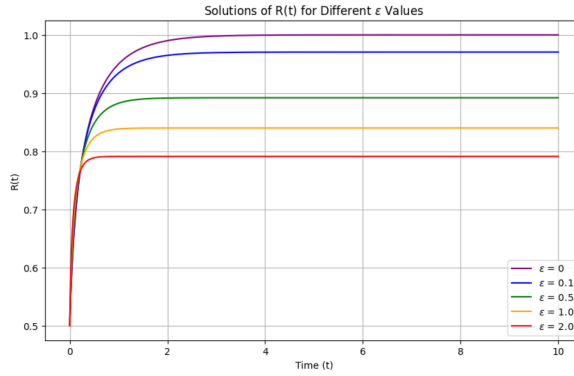


Figure 4.3: Evolution of $R(t)$ with $R_0 = 0.5$ for various ε .

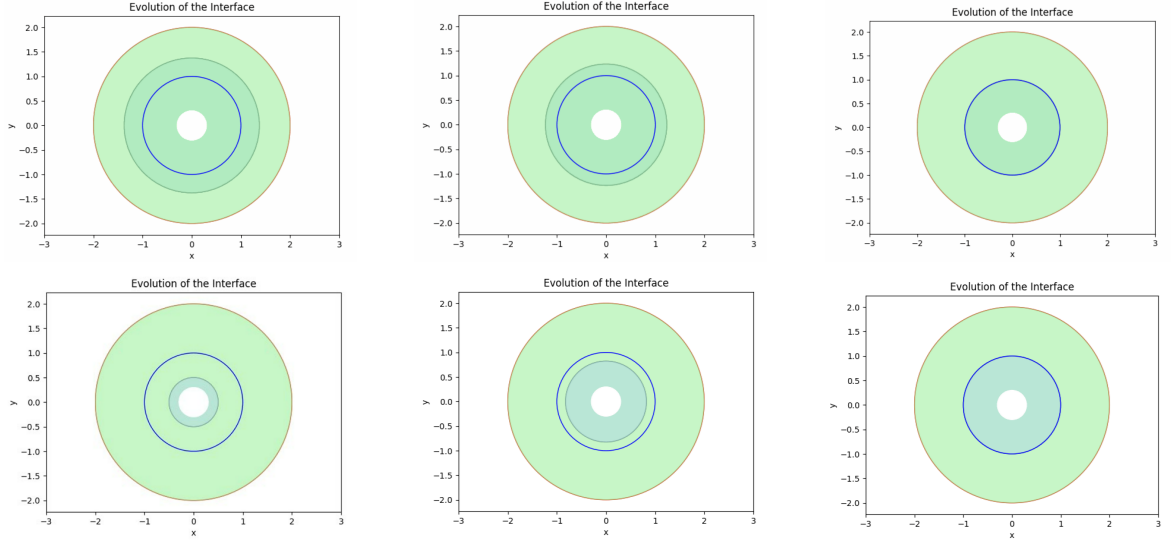


Figure 4.4: Evolution diagram when $\epsilon = 0$

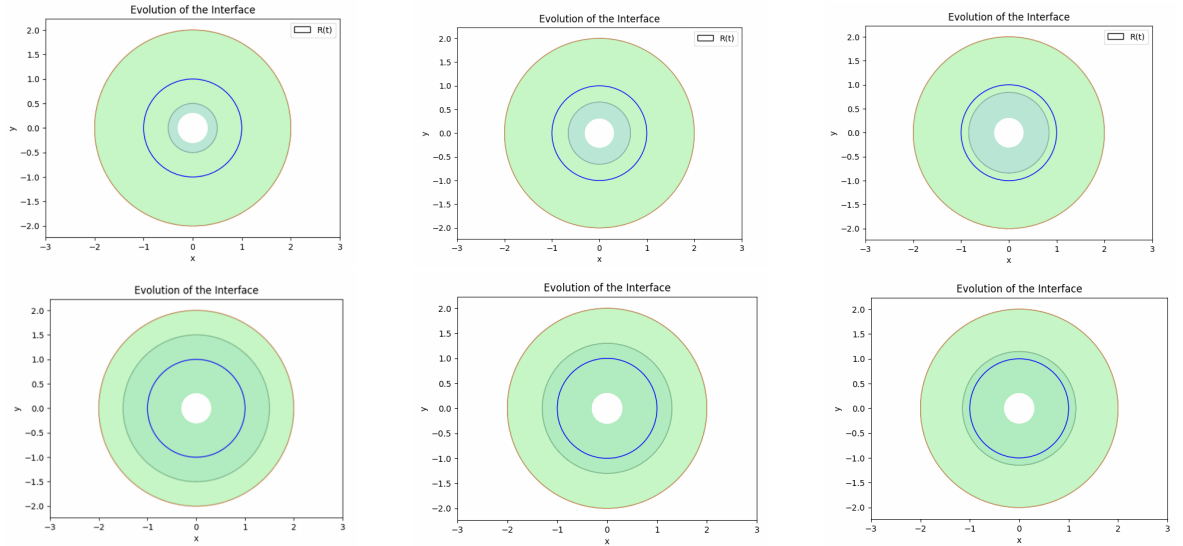


Figure 4.5: Evolution diagram when $\epsilon = 1$

unknown subdomain Ω^+ , enclosed by Γ , corresponds to a region with higher conductivity, modeled by a piecewise constant coefficient:

$$a(x) = \begin{cases} a_1 = 2.0 & \text{in } \Omega^+, \\ a_2 = 1.0 & \text{in } \Omega^- := \Omega \setminus \overline{\Omega^+}. \end{cases} \quad (4.75)$$

We consider two elliptic problems in the composite domain Ω :

- The Dirichlet problem for $w(x)$ with prescribed potential $G = 2.59026$ on the outer boundary $\Gamma_e := \partial B(0, r_{\text{outer}})$ and homogeneous Dirichlet condition on the inner boundary $\Gamma_i := \partial B(0, r_{\text{inner}})$;
- The Neumann problem for $u(x)$ with prescribed normal flux $F = 1.0$ on Γ_e and the same homogeneous Dirichlet data on Γ_i .

The optimization objective is the Kohn–Vogelius-type functional:

$$J(\Gamma) = \int_{\Omega} a(x) |\nabla u(x) - \nabla w(x)|^2 dx, \quad (4.76)$$

which vanishes when the solutions u and w are identical. In the radially symmetric case, the optimal interface is known analytically to be a circle of radius $R^* = 1.0$.

To challenge the symmetry, we initialize the interface with a perturbed radial function:

$$R_0(\theta) = a_0 + \sum_{n=1}^N (a_n \cos(n\theta) + b_n \sin(n\theta)), \quad N = 8, \quad a_0 = 1.2, \quad (4.77)$$

where a_n, b_n are independently sampled from $[-0.05, 0.05]$. This produces a non-circular, oscillatory interface with no rotational symmetry, introducing significant geometric complexity.

At each time step, the domain is triangulated in polar coordinates, adapting to the current interface shape $R(\theta)$. The PDEs are solved via finite element methods, and the shape derivative of J is computed using Hadamard’s formula. Geometric regularization is applied through a combined perimeter and elastica energy:

$$\mathcal{E}(\Gamma) = \int_{\Gamma} ds + \frac{1}{2} \int_{\Gamma} \kappa^2 ds, \quad (4.78)$$

with corresponding shape derivative:

$$d\mathcal{E} = \nabla_s^2 \kappa + \frac{1}{2} \kappa^3 - \kappa, \quad (4.79)$$

where κ is the curvature and ∇_s denotes the arc-length tangential derivative.

The evolution of the interface is governed by the geometric gradient flow:

$$\partial_t f = -\varepsilon \left(\nabla_s^2 \kappa + \frac{1}{2} \kappa^3 - \kappa \right) \mathbf{n} - dJ \cdot \mathbf{n}, \quad (4.80)$$

where $\mathbf{n}$ is the outward unit normal, and $\varepsilon = 0.1$ controls the strength of regularization. The flow is projected onto the radial direction, respecting the polar representation.

Time integration is performed using an explicit time-stepping scheme with step size $\Delta t = 10^{-3}$ for 500 steps. Despite the irregular, perturbed nature of the initial shape, the interface evolves smoothly and stabilizes near a circular configuration. The functional $J(\Gamma)$ decreases significantly during the process, and the final configuration closely matches the true solution with $R \approx R^* = 1.0$.

Figures 4.6, 4.7, and 4.8 illustrate the interface evolution at various time steps, highlighting the progressive regularization and convergence of the shape. The effectiveness of the regularized gradient flow in recovering the optimal interface, even from nonsymmetric and noisy initial data, demonstrates the robustness and accuracy of the proposed method.

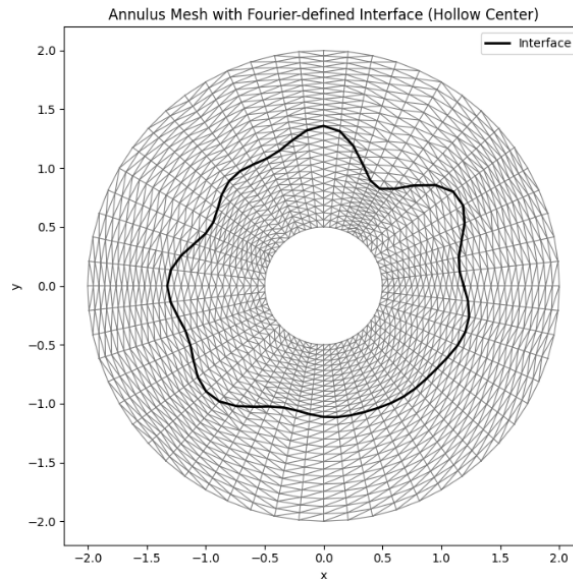


Figure 4.6: Grid division of domain

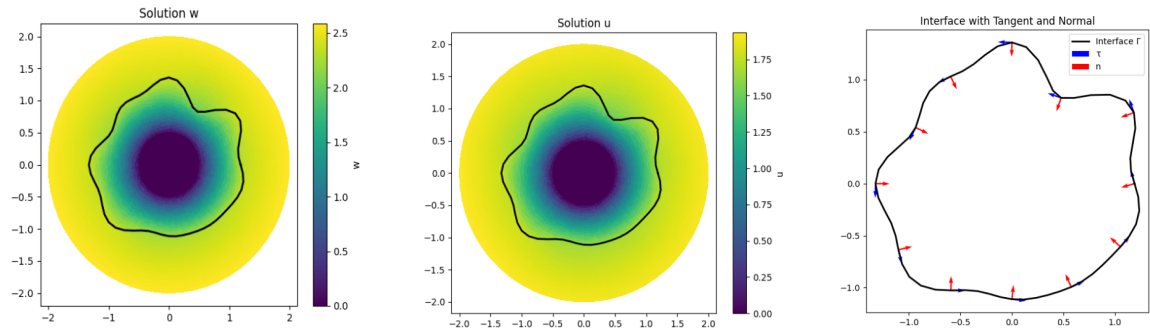


Figure 4.7: Initial distribution of solution w and solution v and normal and tangent vectors on the interface

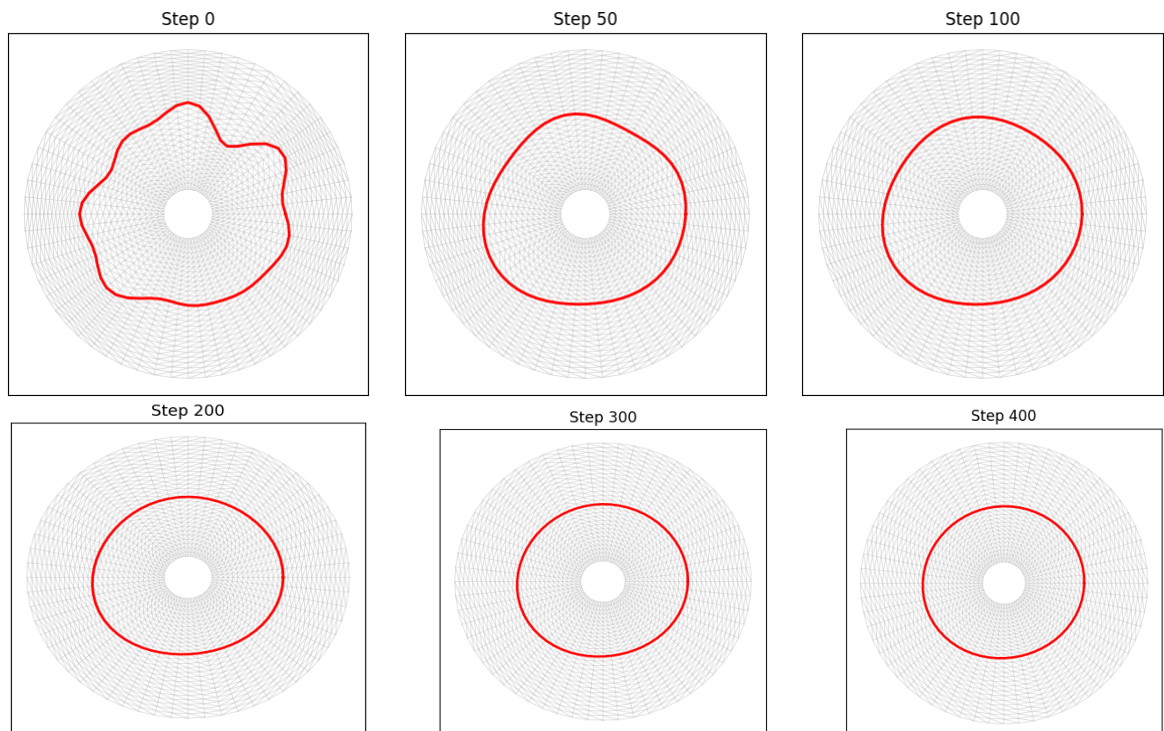


Figure 4.8: Evolution of structural shape during optimization.

4.9 Formulation of an interface identification problem in linear elasticity

We consider an interface identification problem in the setting of linear elasticity, where the objective is to reconstruct or optimize the geometry of an internal interface Γ that separates two materials with distinct elastic properties. The problem is posed on a bounded, smooth domain $D \subset \mathbb{R}^N$ whose boundary is partitioned into $\partial D = \Gamma_i \cup \Gamma_e$. Here, Γ_i denotes a fixed boundary with prescribed Dirichlet conditions, and Γ_e corresponds to the portion where either displacement or traction data are imposed.

The unknown interface Γ divides D into two disjoint subdomains, Ω_1 and Ω_2 , each occupied by different materials. The elastic behavior in each subdomain is described by a piecewise-constant elasticity tensor $\mathbb{C}(x)$, which takes values $\mathbb{C}_1$ in Ω_1 and $\mathbb{C}_2$ in Ω_2 .

To detect or recover the interface, we introduce a Kohn–Vogelius-type discrepancy functional:

$$J(\Gamma) = \frac{1}{2} \int_D \sigma(U - w) : \varepsilon(U - w), dx, \quad (4.81)$$

where U and w are displacement fields arising from two boundary value problems with different boundary data. The strain tensor is defined as $\varepsilon(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$, and the stress tensor is given by $\sigma(u) = \mathbb{C}(x)\varepsilon(u)$.

The displacement field U solves the Dirichlet-driven problem:

$$\begin{cases} -\operatorname{div}(\sigma(U)) = 0 & \text{in } D, \\ U = 0 & \text{on } \Gamma_i, \\ U = N & \text{on } \Gamma_e, \\ \llbracket U \rrbracket = 0, \quad \llbracket \sigma(U) \cdot n \rrbracket = 0 & \text{on } \Gamma. \end{cases} \quad (4.82)$$

The field w solves the Neumann-driven problem:

$$\begin{cases} -\operatorname{div}(\sigma(w)) = 0 & \text{in } D, \\ w = 0 & \text{on } \Gamma_i, \\ \sigma(w) \cdot n = P & \text{on } \Gamma_e, \\ \llbracket w \rrbracket = 0, \quad \llbracket \sigma(w) \cdot n \rrbracket = 0 & \text{on } \Gamma. \end{cases} \quad (4.83)$$

Here, $\llbracket \cdot \rrbracket$ denotes the jump across the interface Γ , and n is the unit normal vector on Γ . The boundary data N and P represent the imposed displacement and traction, respectively, on Γ_e .

The function space for the weak formulation is defined as:

$$\mathcal{V} := v \in H^1(D; \mathbb{R}^N) \mid v = 0 \text{ on } \Gamma_i, \quad (4.84)$$

with $U \in \mathcal{V}_N := v \in \mathcal{V} \mid v = N \text{ on } \Gamma_e$ and $w \in \mathcal{V}_0 := v \in \mathcal{V} \mid v = 0 \text{ on } \Gamma_e$. Under standard assumptions on regularity and coercivity, both problems admit unique weak solutions.

The Kohn–Vogelius functional $J(\Gamma)$ quantifies the difference in elastic response under two types of boundary excitation. By minimizing $J(\Gamma)$, one seeks an interface configuration such that the two solutions match as closely as possible, indicating that the geometry of Γ is consistent with the physical response of the system.

This methodology forms the basis for many inverse problems in mechanics, including interface detection, structural health monitoring, and nondestructive testing. In the following sections, we develop the shape derivative of $J(\Gamma)$ with respect to perturbations of the interface and derive the variational tools necessary for numerical shape optimization.

4.9.1 Shape sensitivity

To compute the first-order shape derivative of the Kohn–Vogelius functional

$$J(\Gamma) = \frac{1}{2} \int_D \sigma(U - w) : \varepsilon(U - w) dx, \quad (4.85)$$

We perturb the interface Γ within a fixed domain $D \subset \mathbb{R}^N$ using a smooth velocity field V . This velocity field generates a family of diffeomorphisms $\{T_t : 0 \leq t \leq \tau\}$ and corresponding perturbed interfaces $\Gamma_t = T_t(\Gamma)$.

At each time t , the perturbed functional is given by

$$J(\Gamma_t) = \frac{1}{2} \int_D \sigma(U_t - w_t) : \varepsilon(U_t - w_t) dx, \quad (4.86)$$

where U_t and w_t are the solutions to the following transmission problems on D with the perturbed interface Γ_t .

Subproblem 1: The displacement field U_t solves

$$\left\{ \begin{array}{ll} -\operatorname{div}(\sigma(U_t)) = 0 & \text{in } D, \\ U_t = 0 & \text{on } \Gamma_i, \\ U_t = N & \text{on } \Gamma_e, \\ \llbracket \sigma(U_t) \cdot n \rrbracket = 0 & \text{on } \Gamma_t, \\ \llbracket U_t \rrbracket = 0 & \text{on } \Gamma_t, \end{array} \right. \quad (4.87)$$

Subproblem 2: The displacement field w_t solves

$$\begin{cases} -\operatorname{div}(\sigma(w_t)) = 0 & \text{in } D, \\ w_t = 0 & \text{on } \Gamma_i, \\ \sigma(w_t) \cdot n = P & \text{on } \Gamma_e, \\ \llbracket \sigma(w_t) \cdot n \rrbracket = 0 & \text{on } \Gamma_t, \\ \llbracket w_t \rrbracket = 0 & \text{on } \Gamma_t. \end{cases} \quad (4.88)$$

Our goal is to compute the shape derivative

$$d\mathcal{J}(0) = \lim_{t \rightarrow 0^+} \frac{J(\Gamma_t) - J(\Gamma)}{t} \quad (4.89)$$

of the functional $\mathcal{J}(t) := J(\Gamma_t)$.

Due to the dependence of the function spaces on the perturbed domain, we apply a standard technique in shape calculus: we pull back all functions to the fixed reference domain D via the diffeomorphisms T_t^{-1} . This reparametrization allows us to define transformed function spaces as

$$H_{\Gamma_i}^1(D_t) = \{\varphi \circ T_t^{-1} : \varphi \in H_{\Gamma_i}^1(D)\}, \quad (4.90)$$

which preserves boundary conditions under the mapping, since T_t is a homeomorphism and maps Γ to Γ_t .

Using this change of variables, we introduce the transformed Kohn-Vogelius functional

$$\tilde{\mathcal{J}}(t, \varphi) = \frac{1}{2} \int_D \sigma(U^t - w^t) : \varepsilon(U^t - w^t) J_t dx, \quad (4.91)$$

where $U^t = U_t \circ T_t$, $w^t = w_t \circ T_t$, and $J_t = |\det DT_t|$ is the Jacobian determinant of the transformation T_t .

Therefore, the shape derivative becomes

$$\mathcal{J}(t) = \tilde{\mathcal{J}}(t, \varphi^t), \quad (4.92)$$

where φ^t minimizes $\tilde{\mathcal{J}}(t, \cdot)$ over the fixed space $H_{\Gamma_i}^1(D)$, and the problem is now formulated on a fixed domain D , facilitating differentiation with respect to t .

Differentiability of the Kohn-Vogelius Functional with Respect to a Shape Perturbation

We now consider the differentiability of the function

$$\mathcal{J}(t) = \inf_{\varphi \in H_{\Gamma_i}^1(D)} \tilde{\mathcal{J}}(t, \varphi), \quad (4.93)$$

with respect to the perturbation parameter t at $t = 0$.

To apply a differentiability result in this setting, we adopt a version of the corresponding theorem, following the approach in Delfour and Zolésio, 2011b; Ito et al., 2008.

Theorem 4.9.1. *Let $\mathcal{V} = H_{\Gamma_i}^1(D)$ be the fixed Sobolev space with homogeneous Dirichlet conditions on Γ_i . Define for each $t \in [0, \tau]$,*

$$g(t) := \inf_{\varphi \in \mathcal{V}} G(t, \varphi), \quad \text{where } G(t, \varphi) := \tilde{J}(t, \varphi). \quad (4.94)$$

Assume the following:

- (H1) *For all $t \in [0, \tau]$, the set of minimizers $X(t) := \{\varphi \in \mathcal{V} : G(t, \varphi) = g(t)\}$ is non-empty.*
- (H2) *For all $\varphi \in \bigcup_{t \in [0, \tau]} X(t)$, the partial derivative $\partial_t G(t, \varphi)$ exists for all $t \in [0, \tau]$.*
- (H3) *There exists a topology $\mathcal{T}_{\mathcal{V}}$ (e.g., weak topology in H^1) such that for any sequence $t_n \rightarrow 0$, there exist a subsequence t_{n_k} , a function $\varphi^0 \in X(0)$, and $\varphi_{n_k} \in X(t_{n_k})$ with:*
 - (i) $\varphi_{n_k} \rightarrow \varphi^0$ in $\mathcal{T}_{\mathcal{V}}$, and
 - (ii) $\liminf_{k \rightarrow \infty} \partial_t G(t_{n_k}, \varphi_{n_k}) \geq \partial_t G(0, \varphi^0)$.
- (H4) *For all $\varphi \in X(0)$, the mapping $t \mapsto \partial_t G(t, \varphi)$ is upper semicontinuous at $t = 0$.*

Then there exists a minimizer $\varphi^0 \in X(0)$ such that:

$$d\mathcal{J}(0) = \lim_{t \searrow 0} \frac{\mathcal{J}(t) - \mathcal{J}(0)}{t} = \inf_{\varphi \in X(0)} \partial_t G(0, \varphi) = \partial_t G(0, \varphi^0). \quad (4.95)$$

Proof. We aim to establish the existence and precise characterization of the directional derivative of the shape-dependent functional $\mathcal{J} : [0, \tau] \rightarrow \mathbb{R}$, defined by

$$\mathcal{J}(t) := \inf_{\varphi \in H_{\Gamma_i}^1(D)} \tilde{J}(t, \varphi), \quad (4.96)$$

where for each $t \in [0, \tau]$, the perturbed Kohn-Vogelius functional $\tilde{J}(t, \cdot)$ is well-defined and Fréchet differentiable with respect to t for fixed φ .

Let us denote the variation

$$\Delta(t) := \mathcal{J}(t) - \mathcal{J}(0), \quad t > 0, \quad (4.97)$$

and consider the corresponding differential quotient $\frac{\Delta(t)}{t}$. Our objective is to evaluate

$$\mathcal{J}'(0) := \lim_{t \searrow 0} \frac{\mathcal{J}(t) - \mathcal{J}(0)}{t}, \quad (4.98)$$

provided the limit exists.

Let $\varphi^0 \in X(0)$, and for each $t > 0$, let $\varphi^t \in X(t)$, where

$$X(t) := \left\{ \varphi \in H_{\Gamma_i}^1(D) : \tilde{J}(t, \varphi) = \mathcal{J}(t) \right\} \quad (4.99)$$

denotes the (possibly non-unique) set of minimizers at time t . By the minimality of φ^t and φ^0 , we immediately obtain the bounds:

$$\tilde{J}(t, \varphi^t) = \mathcal{J}(t) \leq \tilde{J}(t, \varphi^0), \quad \tilde{J}(0, \varphi^t) \geq \mathcal{J}(0) = \tilde{J}(0, \varphi^0). \quad (4.100)$$

Subtracting the second inequality from the first yields the double inequality:

$$\tilde{J}(t, \varphi^t) - \tilde{J}(0, \varphi^t) \leq \Delta(t) \leq \tilde{J}(t, \varphi^0) - \tilde{J}(0, \varphi^0). \quad (4.101)$$

Due to assumption (H2), the map $t \mapsto \tilde{J}(t, \varphi)$ is differentiable for all $\varphi \in \bigcup_{t \in [0, \tau]} X(t)$. Thus, for each fixed $\varphi \in H_{\Gamma_i}^1(D)$, the fundamental theorem of calculus implies that there exist $\theta_t, \alpha_t \in (0, 1)$ such that:

$$\begin{aligned} \tilde{J}(t, \varphi^t) - \tilde{J}(0, \varphi^t) &= t \cdot \partial_t \tilde{J}(\theta_t t, \varphi^t), \\ \tilde{J}(t, \varphi^0) - \tilde{J}(0, \varphi^0) &= t \cdot \partial_t \tilde{J}(\alpha_t t, \varphi^0). \end{aligned} \quad (4.102)$$

Combining (4.101) and (4.102), and dividing both sides by $t > 0$, we obtain the key estimate:

$$\partial_t \tilde{J}(\theta_t t, \varphi^t) \leq \frac{\Delta(t)}{t} \leq \partial_t \tilde{J}(\alpha_t t, \varphi^0). \quad (4.103)$$

We now define the lower and upper Dini derivatives at $t = 0$ as:

$$\underline{d}\mathcal{J}(0) := \liminf_{t \searrow 0} \frac{\Delta(t)}{t}, \quad \bar{d}\mathcal{J}(0) := \limsup_{t \searrow 0} \frac{\Delta(t)}{t}. \quad (4.104)$$

To analyze the lower bound, let $\{t_n\}_{n \in \mathbb{N}}$ be a sequence in $(0, \tau]$ such that $t_n \rightarrow 0$ and

$$\lim_{n \rightarrow \infty} \frac{\Delta(t_n)}{t_n} = \underline{d}\mathcal{J}(0). \quad (4.105)$$

By assumption (H3), there exists a subsequence $\{t_{n_k}\}_{k \in \mathbb{N}}$, a function $\varphi^0 \in X(0)$, and corresponding elements $\varphi_k \in X(t_{n_k})$ such that:

1. $\varphi_k \rightarrow \varphi^0$ in the topology $\mathcal{T}_X$,
2. $\liminf_{k \rightarrow \infty} \partial_t \tilde{J}(t_{n_k}, \varphi_k) \geq \partial_t \tilde{J}(0, \varphi^0)$.

Applying the left-hand inequality of (4.103) to $t = t_{n_k}$, we obtain:

$$\partial_t \tilde{J}(\theta_{t_{n_k}} t_{n_k}, \varphi_k) \leq \frac{\Delta(t_{n_k})}{t_{n_k}}. \quad (4.106)$$

Taking the lower limit as $k \rightarrow \infty$, and invoking semicontinuity from assumption (H3)(ii), we deduce:

$$\partial_t \tilde{J}(0, \varphi^0) \leq \liminf_{k \rightarrow \infty} \frac{\Delta(t_{n_k})}{t_{n_k}} = \underline{d}\mathcal{J}(0). \quad (4.107)$$

This yields:

$$\inf_{\varphi \in X(0)} \partial_t \tilde{J}(0, \varphi) \leq \partial_t \tilde{J}(0, \varphi^0) \leq \underline{d}\mathcal{J}(0). \quad (4.108)$$

On the other hand, the right-hand inequality in (4.103), combined with the upper semicontinuity assumption (H4), implies that:

$$\forall \varphi \in X(0), \quad \partial_t \tilde{J}(0, \varphi) \geq \bar{d}\mathcal{J}(0), \quad \Rightarrow \quad \bar{d}\mathcal{J}(0) \leq \inf_{\varphi \in X(0)} \partial_t \tilde{J}(0, \varphi). \quad (4.109)$$

Consequently, we obtain the chain of inequalities:

$$\inf_{\varphi \in X(0)} \partial_t \tilde{J}(0, \varphi) \leq \underline{d}\mathcal{J}(0) \leq \bar{d}\mathcal{J}(0) \leq \inf_{\varphi \in X(0)} \partial_t \tilde{J}(0, \varphi), \quad (4.110)$$

from which equality follows throughout. In particular, the limit exists and satisfies:

$$\mathcal{J}'(0) = \lim_{t \searrow 0} \frac{\mathcal{J}(t) - \mathcal{J}(0)}{t} = \inf_{\varphi \in X(0)} \partial_t \tilde{J}(0, \varphi) = \partial_t \tilde{J}(0, \varphi^0), \quad (4.111)$$

where $\varphi^0 \in X(0)$ is a minimizer of the derivative functional $\varphi \mapsto \partial_t \tilde{J}(0, \varphi)$ over the minimizing set $X(0)$. $\square$

In our setting, for each sufficiently small $t \geq 0$, the Kohn–Vogelius functional $\mathcal{J}(t)$ admits a unique minimizer φ^t , where

$$\mathcal{J}(t) = \inf_{\varphi \in H_{\Gamma_i}^1(D)} \tilde{J}(t, \varphi), \quad X(t) := \{\varphi^t\}. \quad (4.112)$$

Thus, to apply a differentiability theorem for the infimum of a parameter-dependent functional, it suffices to verify the continuity of the map $t \mapsto \varphi^t$ at $t = 0$ under a suitable topology (e.g., the weak topology of H^1), and to check that assumptions (H1)–(H4) are satisfied.

We assume that the velocity field $V \in C^0([0, \tau]; \mathcal{D}^2(\mathbb{R}^N, \mathbb{R}^N))$, and that the Neumann boundary data $g \in C^1(\Gamma_e)$. We further suppose that $\tau > 0$ is small enough such that:

$$J_t := \det(DT_t) > 0, \quad \text{and} \quad A(t) := J_t[DT_t]^{-1\top}[DT_t]^{-1} \quad (4.113)$$

satisfy a uniform ellipticity condition: there exist constants $0 < \alpha < \beta$ such that for all $t \in [0, \tau]$ and all symmetric matrices $\xi \in \mathbb{R}_{\text{sym}}^{N \times N}$,

$$\alpha \|\xi\|^2 \leq \mathbb{A}_i(x)\xi : \xi \leq \beta \|\xi\|^2, \quad \text{and} \quad \alpha \leq J_t(x) \leq \beta, \quad \text{for } i = 1, 2. \quad (4.114)$$

The bilinear form associated with the variational formulation of the elasticity problem remains uniformly coercive in $H_{\Gamma_i}^1(D)$, and the Neumann boundary term involving g defines a continuous linear functional. Hence, by the Lax–Milgram lemma, the solution exists uniquely. Setting $\varphi^t := U^t - w^t$, we have that for all $t \in [0, \tau]$, the minimizer exists and is unique, i.e.,

$$X(t) = \{\varphi^t\} \neq \emptyset. \quad (4.115)$$

Thus, assumption (H1) is satisfied.

We now verify assumption (H2). Consider the reparametrized functional:

$$\tilde{J}(t, \varphi) := \frac{1}{2} \sum_{i=1}^2 \int_{\Omega_i} \mathbb{A}_i \varepsilon(\varphi) : \varepsilon(\varphi) \cdot J_t dx. \quad (4.116)$$

Here $\varphi = U^t - w^t$, where $U^t = U_t \circ T_t$, $w^t = w_t \circ T_t$, and the deformation is governed by the velocity field V .

$$\mathbb{A}(x) = \begin{cases} \mathbb{A}_1 & x \in \Omega_1 \\ \mathbb{A}_2 & x \in \Omega_2 \end{cases} \quad (4.117)$$

The tensorial derivative of the transformation is defined as:

$$A'(t) := (\operatorname{div} V_t)I - (DV_t)^\top - DV_t, \quad \text{with } V_t(x) := V(t, T_t(x)). \quad (4.118)$$

Then the shape derivative of the functional can be expressed as:

$$\begin{aligned} \partial_t \tilde{J}(t, \varphi) = & \frac{1}{2} \sum_{i=1}^2 \int_{D_i} \left[A'(t) \varepsilon(\varphi) : \mathbb{A}_i \varepsilon(\varphi) \right. \\ & \left. + \operatorname{div} V_t \cdot \mathbb{A}_i \varepsilon(\varphi) : \varepsilon(\varphi) \right] dx + \int_{\Gamma_e} P \cdot \varphi \cdot (V \cdot n) ds. \end{aligned} \quad (4.119)$$

Since P is fixed, V is smooth, and φ is fixed in the variational sense, all the terms above depend smoothly on t . Therefore, the map $t \mapsto \tilde{J}(t, \varphi)$ is differentiable in $[0, \tau]$ for every fixed $\varphi \in H_{\Gamma_i}^1(D)$, and assumption (H2) holds.

As each $X(t)$ is a singleton $\{\varphi^t\}$, to verify assumption (H3), it suffices to show the continuity of $t \mapsto \varphi^t$ with respect to the weak topology in $H_{\Gamma_i}^1(D)$. From standard elliptic regularity and compactness results, and the stability of the variational solution with respect to domain deformation, we conclude that $\varphi^t \rightharpoonup \varphi^0 \in X(0)$ weakly in H^1 , as $t \rightarrow 0$. Moreover, the weak lower semicontinuity of the functional derivative and the continuity of the geometry imply:

$$\liminf_{t \rightarrow 0} \partial_t \tilde{J}(t, \varphi^t) \geq \partial_t \tilde{J}(0, \varphi^0), \quad (4.120)$$

which verifies assumption (H3).

Finally, for (H4), since for each fixed $\varphi \in X(0)$, the expression $\partial_t \tilde{J}(t, \varphi)$ depends smoothly on T_t , V , and the coefficients $\mathbb{A}_i$, and all these components are regular in t , it follows that the map $t \mapsto \partial_t \tilde{J}(t, \varphi)$ is upper semicontinuous at $t = 0$, hence (H4) is satisfied.

Therefore, all conditions (H1)–(H4) of the differentiability theorem are fulfilled, and we conclude:

$$\mathcal{J}'(0) = \lim_{t \rightarrow 0^+} \frac{\mathcal{J}(t) - \mathcal{J}(0)}{t} = \inf_{\varphi \in X(0)} \partial_t \tilde{J}(0, \varphi) = \partial_t \tilde{J}(0, \varphi^0), \quad (4.121)$$

where φ^0 is the unique minimizer of $\tilde{J}(0, \cdot)$, and also minimizes the shape derivative functional $\varphi \mapsto \partial_t \tilde{J}(0, \varphi)$.

To prove the strong continuity of the minimizer, we consider the variational equations satisfied by U^t and w^t . For $\varphi^t := U^t - w^t$, we subtract the perturbed problem at $t > 0$ from that at $t = 0$. For all test functions $\psi \in H_{\Gamma_i}^1(D)$, one has:

$$\int_D A(t) \varepsilon(\varphi^t) : \mathbb{A} \varepsilon(\psi) dx = \int_{\Gamma_e} P \cdot \psi \cdot J_t ds, \quad (4.122)$$

whereas at $t = 0$, the limit function $\varphi^0 = U^0 - w^0$ satisfies:

$$\int_D \varepsilon(\varphi^0) : \mathbb{A} \varepsilon(\psi) dx = \int_{\Gamma_e} P \cdot \psi ds. \quad (4.123)$$

Subtracting and taking $\psi = \varphi^t - \varphi^0$, we obtain:

$$\begin{aligned} \int_D |\varepsilon(\varphi^t - \varphi^0)|^2 dx &= - \int_D (A(t) - I) \varepsilon(\varphi^t) : \mathbb{A} \varepsilon(\varphi^t - \varphi^0) dx \\ &\quad + \int_{\Gamma_e} P \cdot (\varphi^t - \varphi^0)(J_t - 1) ds. \end{aligned} \quad (4.124)$$

Applying Hölder's inequality and the boundedness of φ^t in H^1 , we obtain:

$$\|\varphi^t - \varphi^0\|_{H^1(D)} \leq C (\|A(t) - I\|_{L^\infty} + \|J_t - 1\|_{L^\infty}), \quad (4.125)$$

and since $A(t) \rightarrow I$ and $J_t \rightarrow 1$ uniformly as $t \rightarrow 0$, we conclude:

$$\varphi^t \rightarrow \varphi^0 \quad \text{strongly in } H_{\Gamma_i}^1(D), \quad (4.126)$$

thus verifying assumption (H3)(i) in the strong topology.

We now verify assumption (H3)(ii). For any fixed $\varphi \in H_{\Gamma_i}^1(D)$, the shape derivative of the reparametrized functional reads:

$$\begin{aligned} \partial_t \tilde{J}(t, \varphi) &= \frac{1}{2} \sum_{i=1}^2 \int_{\Omega_i} A'(t) \varepsilon(\varphi) : \mathbb{A}_i \varepsilon(\varphi) \, dx \\ &\quad + \frac{1}{2} \sum_{i=1}^2 \int_{\Omega_i} (\operatorname{div} V_t) \cdot \mathbb{A}_i \varepsilon(\varphi) : \varepsilon(\varphi) \, dx \\ &\quad + \int_{\Gamma_e} P \cdot \varphi \cdot \operatorname{div}_{\Gamma} V \, ds. \end{aligned} \quad (4.127)$$

Letting $t \rightarrow 0$ and using the regularity of V and the strong convergence $\varphi^t \rightarrow \varphi^0$ in H^1 , we split:

$$\begin{aligned} &\partial_t \tilde{J}(t, \varphi^t) - \partial_t \tilde{J}(0, \varphi^0) \\ &= \frac{1}{2} \int_D (A'(t) - A'(0)) \varepsilon(\varphi^t) : \mathbb{A} \varepsilon(\varphi^t) \, dx \\ &\quad + \frac{1}{2} \int_D A'(0) (\varepsilon(\varphi^t) : \mathbb{A} \varepsilon(\varphi^t) - \varepsilon(\varphi^0) : \mathbb{A} \varepsilon(\varphi^0)) \, dx \\ &\quad + \int_{\Gamma_e} P \cdot (\varphi^t (J_{\Gamma, t} - 1) + (\varphi^t - \varphi^0)) \, ds. \end{aligned} \quad (4.128)$$

By strong convergence, boundedness, and smoothness of coefficients, each term vanishes as $t \rightarrow 0$, yielding:

$$\liminf_{t \rightarrow 0} \partial_t \tilde{J}(t, \varphi^t) \geq \partial_t \tilde{J}(0, \varphi^0), \quad (4.129)$$

thus verifying (H3)(ii).

Finally, assumption (H4) follows since for fixed $\varphi \in H_{\Gamma_i}^1(D)$, the mapping

$$t \mapsto \partial_t \tilde{J}(t, \varphi) \quad (4.130)$$

is continuous on $[0, \tau]$, as all involved terms— $A'(t)$, $\sigma(\varphi)$, and J_t —depend smoothly on t under our regularity assumptions on the velocity field V . Therefore, all assumptions (H1)–(H4) of Theorem 4.9.1 are satisfied.

As a consequence, for any admissible velocity field $V \in C^0([0, \tau]; \mathcal{D}^2(\mathbb{R}^N, \mathbb{R}^N))$, we have the first-order shape derivative of the Kohn–Vogelius functional:

$$d\mathcal{J}(0; V) = \int_D \frac{1}{2} A'(0) \varepsilon(\varphi^0) : \mathbb{A} \varepsilon(\varphi^0) \, dx + \int_{\Gamma_e} g \cdot \varphi^0 \cdot \operatorname{div}_{\Gamma} V \, ds, \quad (4.131)$$

where $\varphi^0 = U^0 - w^0$ is the difference of the state solutions at $t = 0$.

Now, we seek to express this volume shape derivative as an interface (Hadamard) form. Since only the interface Γ is variable while the outer boundaries Γ_i and Γ_e remain fixed, we note that $\operatorname{div}_\Gamma V = 0$ on Γ_e , so the second integral vanishes.

Although the first term appears as a volume integral over D , the perturbation of the domain affects only the interface Γ , where the material tensor $\mathbb{A}(x)$ jumps. As a result, the shape derivative localizes to the interface in the sense of distributions.

By the Hadamard structure theorem (see e.g., Sokolowski and Zolesio, 1992), for any smooth test function ψ , we have:

$$\int_D A'(0) \psi(x) dx = \int_\Gamma \llbracket \psi \rrbracket (V \cdot n) ds, \quad (4.132)$$

where $\llbracket \cdot \rrbracket$ denotes the jump across the interface Γ from Ω_1 to Ω_2 .

Recalling that $\mathbb{A}(x)$ is piecewise constant, given by:

$$\mathbb{A}(x) = \begin{cases} \mathbb{A}_1, & x \in \Omega_1, \\ \mathbb{A}_2, & x \in \Omega_2, \end{cases} \quad (4.133)$$

we apply the Hadamard structure to obtain the interface representation:

$$\int_D \frac{1}{2} A'(0) \varepsilon(\varphi^0) : \mathbb{A}(x) \varepsilon(\varphi^0) dx = \int_\Gamma \frac{1}{2} \llbracket \mathbb{A} \varepsilon(\varphi^0) : \varepsilon(\varphi^0) \rrbracket (V \cdot n) ds. \quad (4.134)$$

Therefore, the first-order shape derivative becomes:

$$d\mathcal{J}(0; V) = \int_\Gamma \frac{1}{2} \llbracket \mathbb{A} \varepsilon(\varphi^0) : \varepsilon(\varphi^0) \rrbracket (V \cdot n) ds. \quad (4.135)$$

In the case of isotropic linear elasticity, the stress tensor is given by

$$\sigma(\varphi) = \mathbb{A} \varepsilon(\varphi), \quad \text{with } \varepsilon(\varphi) = \frac{1}{2} (\nabla \varphi + \nabla \varphi^\top). \quad (4.136)$$

Hence, the shape derivative can be equivalently written as:

$$d\mathcal{J}(0; V) = \int_\Gamma \frac{1}{2} \llbracket \sigma(\varphi^0) : \varepsilon(\varphi^0) \rrbracket (V \cdot n) ds, \quad (4.137)$$

where the jump $\llbracket \cdot \rrbracket$ is understood as:

$$\llbracket \sigma(\varphi^0) : \varepsilon(\varphi^0) \rrbracket = \sigma_1(\varphi^0) : \varepsilon(\varphi^0) - \sigma_2(\varphi^0) : \varepsilon(\varphi^0), \quad (4.138)$$

with $\sigma_i(\varphi^0) = \mathbb{A}_i \varepsilon(\varphi_i^0)$ for $i = 1, 2$.

This concludes the Hadamard structure formula for the shape derivative of the Kohn–Vogelius functional under interface perturbations.

Lemma 4.9.2. *Assume that $V \in C^0([0, \tau]; \mathcal{D}^1(\mathbb{R}^N, \mathbb{R}^N))$ is an admissible velocity field, and that the Neumann boundary data $P \in L^2(\Gamma_e)$ is fixed. Then for all $\varphi \in H^1(D)$, the pullbacks satisfy strong convergence:*

$$\lim_{t \searrow 0} \varphi \circ T_t = \varphi, \quad \text{and} \quad \lim_{t \searrow 0} \varphi \circ T_t^{-1} = \varphi \quad \text{in } H^1(D). \quad (4.139)$$

Moreover, the difference $\varphi^t := U^t - w^t$ between the Dirichlet and Neumann solutions of the elasticity system remains uniformly bounded:

$$\exists C > 0 \quad \text{such that} \quad \sup_{t \in [0, \tau]} \|\varphi^t\|_{H_{\Gamma_i}^1(D)} \leq C. \quad (4.140)$$

Proof. Let $\varphi \in H^1(D)$ be arbitrary. Since $\mathcal{D}^1(D)$ is dense in $H^1(D)$, for any $\varepsilon > 0$, there exists $\varphi_\varepsilon \in \mathcal{D}^1(D)$ such that:

$$\|\varphi - \varphi_\varepsilon\|_{H^1(D)} < \varepsilon. \quad (4.141)$$

We decompose the difference:

$$\|\varphi \circ T_t - \varphi\|_{H^1(D)} \leq \|\varphi \circ T_t - \varphi_\varepsilon \circ T_t\| + \|\varphi_\varepsilon \circ T_t - \varphi_\varepsilon\| + \|\varphi_\varepsilon - \varphi\|. \quad (4.142)$$

The first and third terms are bounded by ε since composition with T_t preserves the H^1 norm:

$$\|\varphi \circ T_t - \varphi_\varepsilon \circ T_t\|_{H^1(D)} = \|\varphi - \varphi_\varepsilon\|_{H^1(D)}. \quad (4.143)$$

For the middle term, note that φ_ε is smooth and compactly supported, hence Lipschitz. Using the fact that $T_t(x) = x + tV(x) + o(t)$, we obtain:

$$\|\varphi_\varepsilon \circ T_t - \varphi_\varepsilon\|_{H^1(D)} \leq Ct. \quad (4.144)$$

Thus,

$$\|\varphi \circ T_t - \varphi\|_{H^1(D)} \leq 2\varepsilon + Ct. \quad (4.145)$$

Letting $t \rightarrow 0$ and then $\varepsilon \rightarrow 0$ shows strong convergence in $H^1(D)$.

The convergence of $\varphi \circ T_t^{-1} \rightarrow \varphi$ follows similarly by change of variables:

$$\int_D |\varphi \circ T_t^{-1} - \varphi|^2 dx = \int_D |\varphi(x) - \varphi \circ T_t(x)|^2 J_t^{-1}(x) dx, \quad (4.146)$$

and since $J_t^{-1} \rightarrow 1$ uniformly, the result follows.

Now define $\varphi^t := U^t - w^t$ as the difference of solutions to the Dirichlet and Neumann elasticity problems. After pullback to the reference domain D , the associated bilinear form is:

$$a_t(u, v) := \int_D \mathbb{A}^t(x) \varepsilon(u) : \varepsilon(v) J_t(x) dx, \quad (4.147)$$

where $\mathbb{A}^t(x)$ is the (piecewise constant) elasticity tensor after transformation, and $J_t(x)$ is the Jacobian determinant of T_t .

The variational formulations are:

$$\begin{aligned} a_t(U^t, v) &= 0, \\ a_t(w^t, v) &= \int_{\Gamma_e} P \cdot v \, ds, \quad \forall v \in H_{\Gamma_i}^1(D). \end{aligned}$$

Subtracting yields:

$$a_t(\varphi^t, v) = - \int_{\Gamma_e} P \cdot v \, ds. \quad (4.148)$$

By ellipticity, we have:

$$a_t(v, v) \geq \alpha \|v\|_{H_{\Gamma_i}^1(D)}^2 \quad \text{for some } \alpha > 0, \quad (4.149)$$

uniformly in t . Moreover, the right-hand side satisfies:

$$\left| \int_{\Gamma_e} P \cdot v \, ds \right| \leq \|P\|_{L^2(\Gamma_e)} \cdot \|v\|_{L^2(\Gamma_e)} \leq C \|v\|_{H^1(D)}, \quad (4.150)$$

by trace inequality. Hence, the functional is bounded in $H^{-1}(D)$.

From the Lax–Milgram theorem, the solution φ^t exists uniquely and satisfies:

$$\|\varphi^t\|_{H_{\Gamma_i}^1(D)} \leq \frac{1}{\alpha} \cdot \sup_{\|v\|_{H_{\Gamma_i}^1(D)}=1} \left| \int_{\Gamma_e} P \cdot v \, ds \right| \leq C, \quad (4.151)$$

with C independent of t . This completes the proof. $\square$

4.9.2 Geometric gradient flow for interface evolution

To describe the time evolution of the unknown interface Γ , we adopt a geometric gradient flow approach. The interface is modeled as a smooth, closed curve embedded in $\mathbb{R}^2$, represented by a regular parametrization:

$$\Gamma = f(\theta), \quad \theta \in \mathbb{S}^1, \quad (4.152)$$

where $f : \mathbb{S}^1 \rightarrow \mathbb{R}^2$ is a 2π -periodic immersion. Here, $\mathbb{S}^1$ denotes the unit circle, interpreted as the quotient space $\mathbb{R}/2\pi\mathbb{Z}$.

The arc length element along the curve is given by:

$$ds = \sqrt{g(\theta)} \, d\theta, \quad \text{with } g(\theta) = |\partial_\theta f(\theta)|^2, \quad (4.153)$$

where $g(\theta)$ serves as the local metric coefficient (first fundamental form). Differentiation with respect to arc length is then defined as:

$$\partial_s = \frac{1}{\sqrt{g}} \partial_\theta. \quad (4.154)$$

Assuming the curve is traversed counterclockwise (i.e., increasing θ), we define key geometric quantities:

$$\text{Tangent vector: } \tau(\theta) = \partial_s f = \frac{\partial_\theta f}{|\partial_\theta f|}, \quad (4.155)$$

$$\text{Inward unit normal: } n(\theta) = \tau^\perp = (-\tau_2, \tau_1), \quad (4.156)$$

$$\text{Curvature vector: } k(\theta) = \partial_s \tau = \partial_s^2 f. \quad (4.157)$$

The curvature vector k is orthogonal to the tangent and points in the direction of the normal.

We now introduce two geometric functionals associated with Γ :

- The elastic energy, which penalizes curvature variations:

$$\mathcal{E}_e = \int_\Gamma \frac{1}{2} |k|^2, ds, \quad (4.158)$$

- The perimeter (or total length) of the interface:

$$\mathcal{L} = \int_\Gamma ds = \int_0^{2\pi} \sqrt{g(\theta)} d\theta. \quad (4.159)$$

The total geometric energy functional is the sum:

$$\mathcal{E}(f) = \mathcal{E}_e + \mathcal{L} = \int_\Gamma \left(\frac{1}{2} |k|^2 + 1 \right) ds. \quad (4.160)$$

To evolve the interface, we consider two types of gradient flows:

- An unregularized flow, driven purely by the shape gradient of a variational objective functional J (such as the Kohn–Vogelius functional):

$$\partial_t f + dJ = 0, \quad f(0) = f_0, \quad (4.161)$$

- A regularized flow, where geometric energies are incorporated to ensure smoothness and stability:

$$\partial_t f + \varepsilon(d\mathcal{E}) + dJ = 0, \quad f(0) = f_0, \quad (4.162)$$

where $\varepsilon > 0$ controls the strength of regularization, and $d\mathcal{E}$ denotes the shape gradient of the total geometric energy.

In terms of curvature, the regularization term expands as:

$$d\mathcal{E} = \nabla_s^2 k + \frac{1}{2}|k|^2 k - k, \quad (4.163)$$

leading to the fully regularized flow:

$$\partial_t f + \varepsilon \left(\nabla_s^2 k + \frac{1}{2}|k|^2 k - k \right) + dJ = 0. \quad (4.164)$$

This flow describes the evolution of the interface in the direction of steepest descent for the total energy $\mathcal{J}(f) = J(f) + \varepsilon \mathcal{E}(f)$, and serves as a foundation for numerically stable shape optimization algorithms.

4.9.3 Numerical examples

Example 4.9.1. *We consider a two-dimensional elastic annulus, defined as the domain $D = B_{b_1}(0) \setminus \overline{B_a(0)}$, where the outer radius $b_1 = 1.0$ is fixed, and the inner radius $a \in (0.11, 0.99)$ is the shape parameter to be optimized. The material is assumed to be isotropic and linearly elastic, with Young's modulus $E = 1.0$ and Poisson's ratio $\nu = 0.3$. The corresponding Lamé parameters are given by:*

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)}. \quad (4.165)$$

The shape optimization is formulated through a Kohn–Vogelius type objective functional:

$$\mathcal{J}(a) = \frac{1}{2} \int_D \sigma(U - w) : \varepsilon(U - w) dx, \quad (4.166)$$

where U and w are the displacement solutions to two distinct boundary value problems:

- *The field U satisfies a Neumann boundary condition on the inner boundary (with prescribed traction q) and a prescribed radial displacement $\hat{u}_r$ on the outer boundary, computed from analytical elasticity theory;*
- *The field w is subject to the same Neumann condition q on the inner boundary, but the outer boundary is loaded by a uniform radial traction p_1 .*

This functional measures the discrepancy between the two displacement fields and can be interpreted as a misfit indicator for implicit interface identification.

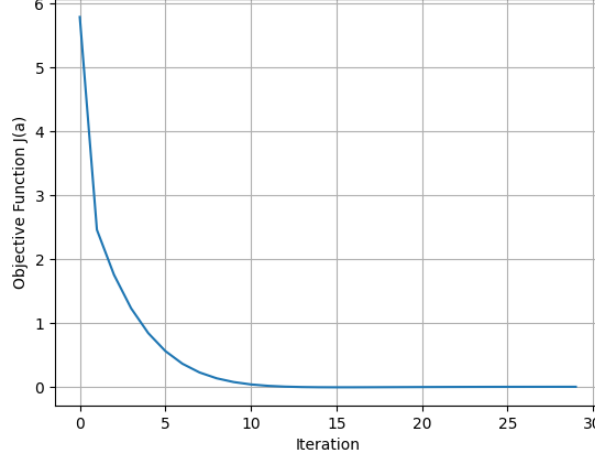


Figure 4.9: Objective function convergence graph

In this experiment, we assume that the interface Γ remains circular throughout the optimization process. Therefore, the shape variable reduces to a single scalar parameter—the inner radius a . This radial symmetry simplifies the problem and allows us to track only the evolution of a while the interface geometry is kept circular.

For the numerical implementation, we use the FEniCS platform and the "mshr" module to generate finite element meshes for each annular configuration. The domain is discretized using quadratic Lagrange vector elements ($\mathbb{P}_2$), and the corresponding weak forms are solved for u and w using standard finite element methods. To optimize the radius a , we adopt a gradient flow approach. Due to radial symmetry, the inner boundary remains circular, so the optimization reduces to a scalar variable.

During the optimization process, the inner radius $a^{(k)}$ and the objective value $\mathcal{J}(a^{(k)})$ are recorded at each iteration. Visualizations of the evolving inner boundary are generated along with the convergence history of the objective functional. The results demonstrate that the shape evolution converges toward a steady optimal radius as shown in Fig 4.10, with monotonic decrease in the objective function as shown in Fig 4.9.

This numerical experiment confirms the effectiveness of the proposed approach in a simplified radially symmetric setting and provides a basis for extending the method to more general interface shapes.

Example 4.9.2. This section presents numerical experiments for the proposed interface reconstruction method applied to a two-dimensional linear elasticity problem. The computational domain is a concentric annular region $D = B_{r_{\max}} \setminus B_{r_{\min}}$, with inner

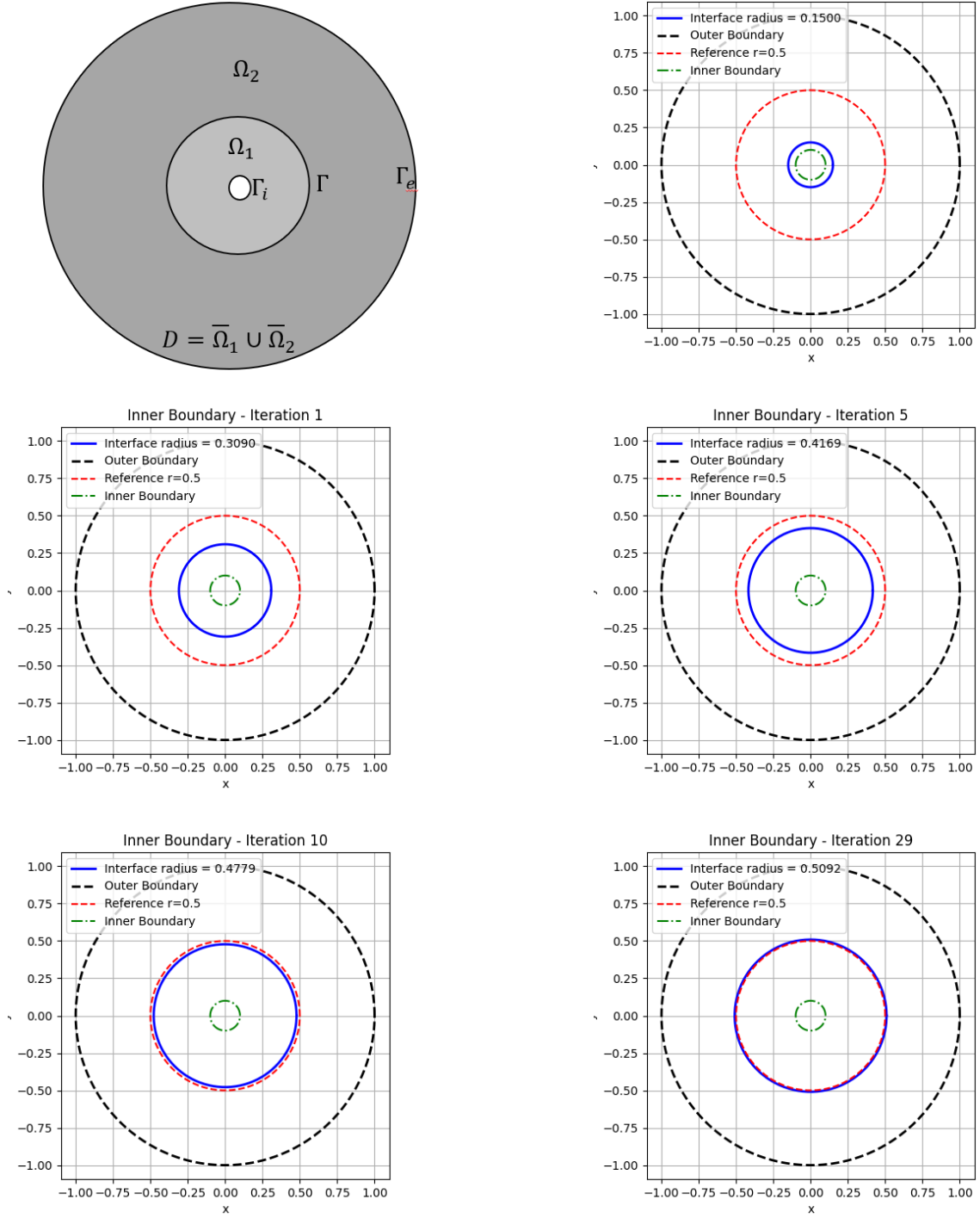


Figure 4.10: Evolution diagram when $\epsilon = 1 \times 10^{-3}$

radius $r_{\min} = 0.3$ and outer radius $r_{\max} = 2.0$. An unknown interface Γ is embedded inside the domain, dividing it into two subregions Ω_1 and Ω_2 with material coefficients $a_1 = 1.0$ and $a_2 = 10.0$, respectively. The interface Γ is represented by a Fourier series of the form

$$r(\theta) = R_0 + \sum_{n=1}^N (a_n \cos(n\theta) + b_n \sin(n\theta)), \quad (4.167)$$

where the reference radius is $R_0 = 1.15$, and the Fourier coefficients a_n, b_n are generated by multiplying decaying exponentials with standard Gaussian noise. This results in an interface that is smooth and nearly circular but not exactly a circle. We set the number of modes to $N = 20$ and the amplitude scaling to $\text{amp} = 0.02$ to ensure regularity.

We consider two state fields u and v , which solve elliptic PDEs under different boundary conditions. The field u satisfies Dirichlet boundary conditions: $u = 0$ on the inner boundary and $u = x + y + 1$ on the outer boundary. The field v satisfies the same Dirichlet condition on the inner boundary, but a Neumann condition on the outer boundary. The Neumann data $N(\theta)$ is generated from an auxiliary program where the interface is fixed as a circle of radius $R = 1$. The corresponding solution u is computed, and its normal derivative on the outer boundary (scaled by a_2) is saved into a file for use as the Neumann input in the main optimization loop. This setup ensures consistency and provides a controlled environment for shape recovery.

The objective functional we seek to minimize is the Kohn–Vogelius-type energy:

$$\mathcal{J}(\Gamma) = \frac{1}{2} \int_D \sigma(u - w) : \varepsilon(u - w) dx, \quad (4.168)$$

which quantifies the difference in energy between the two state fields. We discretize the domain using finite elements in polar coordinates. The angular resolution is set to $N_\theta = 128$, with 6 radial layers in both subdomains. Piecewise linear triangular elements are used, and the resulting linear systems are solved using sparse solvers.

To update the interface, we employ a gradient flow evolution guided by the shape derivative of the functional. To regularize the geometry, we introduce a curvature-based smoothing term $\varepsilon(\partial_s^2 k + \frac{1}{2}k^3 - k)$, where k is the curvature and $\partial_s^2 k$ is its second derivative along arc length. The regularization weight is chosen as $\varepsilon = 10^{-2}$. The interface update is performed in the Fourier coefficient space via FFT decomposition of the radial function.

The evolution runs for 290 time steps with time step size $\Delta t = 10^{-3}$. We track the energy functional $\mathcal{J}$ over iterations and visualize the evolving interface every 20 steps as shown in Figure. 4.12. The results show a consistent decrease in the objective value

and a gradual stabilization of the interface into a smooth shape. The final interface remains noncircular but nearly round, and the objective value is significantly reduced, demonstrating convergence and efficiency of the method.

In addition, we present plots of the numerical solutions u and v , the initial meshe, and the convergence history of the functional as showned in Figure. 4.11. The experiment confirms that our method achieves accurate shape reconstruction while preserving geometric regularity, and offers a promising numerical approach for inverse problems in heterogeneous materials and elasticity interface identification.

4.10 Interface evolution for elastic contact problems via compliance optimization

Building on the geometric framework for interface evolution, we now consider a shape optimization problem arising in linear elasticity with unilateral contact constraints. In this setting, the goal is to determine the optimal shape of an interface Γ such that the total elastic energy—known as the compliance functional—is minimized, subject to boundary conditions and a non-penetration constraint along a designated contact boundary.

Let $D \subset \mathbb{R}^2$ be a bounded elastic body with Lipschitz boundary, decomposed into four disjoint parts:

$$\partial D = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_C, \quad (4.169)$$

where:

- Γ_1 is the Neumann boundary where surface forces P are applied,
- Γ_2 is traction-free,
- Γ_3 is clamped (Dirichlet fixed),
- Γ_C is a potential contact region, where unilateral contact with a rigid obstacle may occur.

We consider the following variational inequality model of linear elasticity with

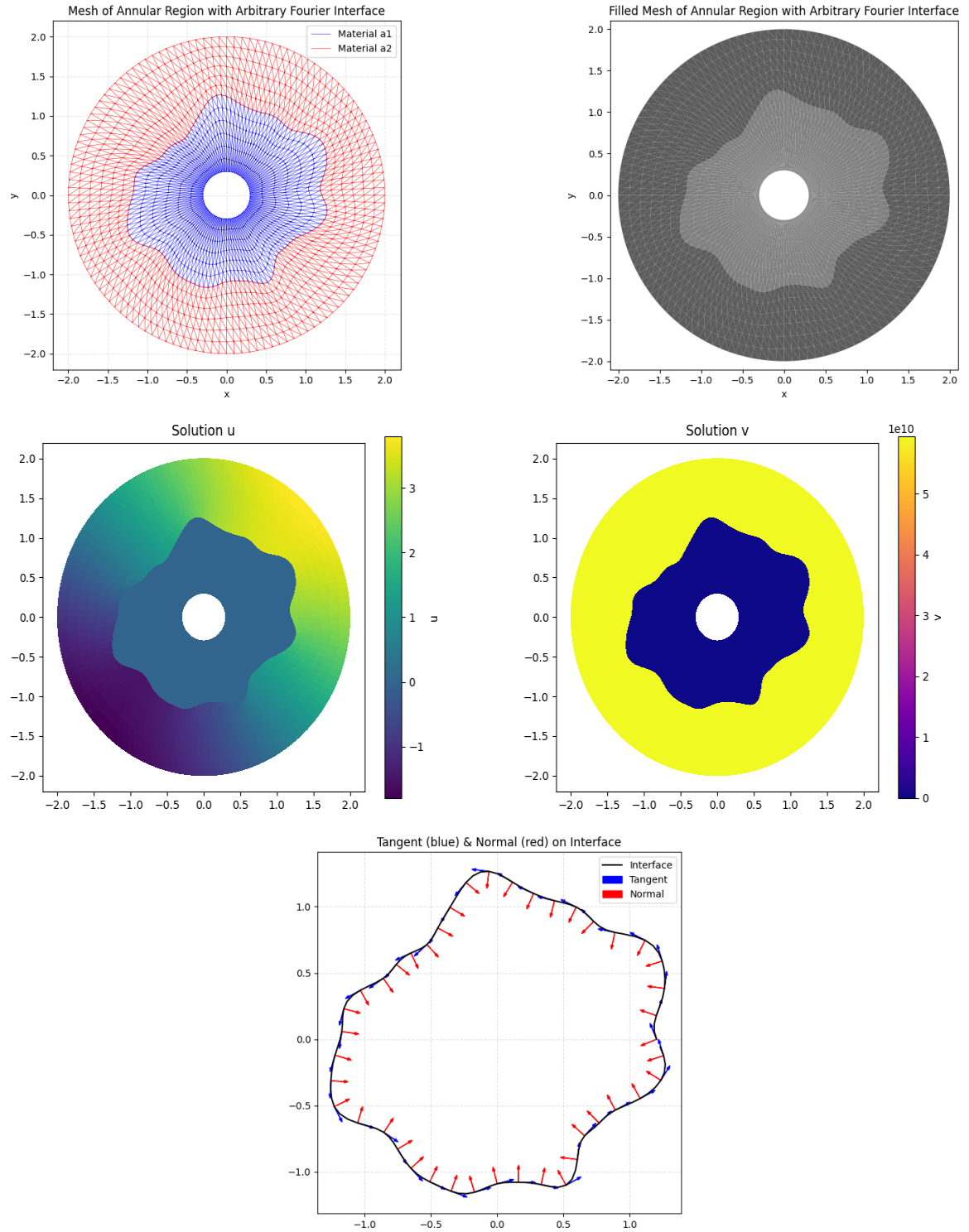


Figure 4.11: Visualization of the initial configuration for the interface reconstruction problem in a two-dimensional elastic annulus.

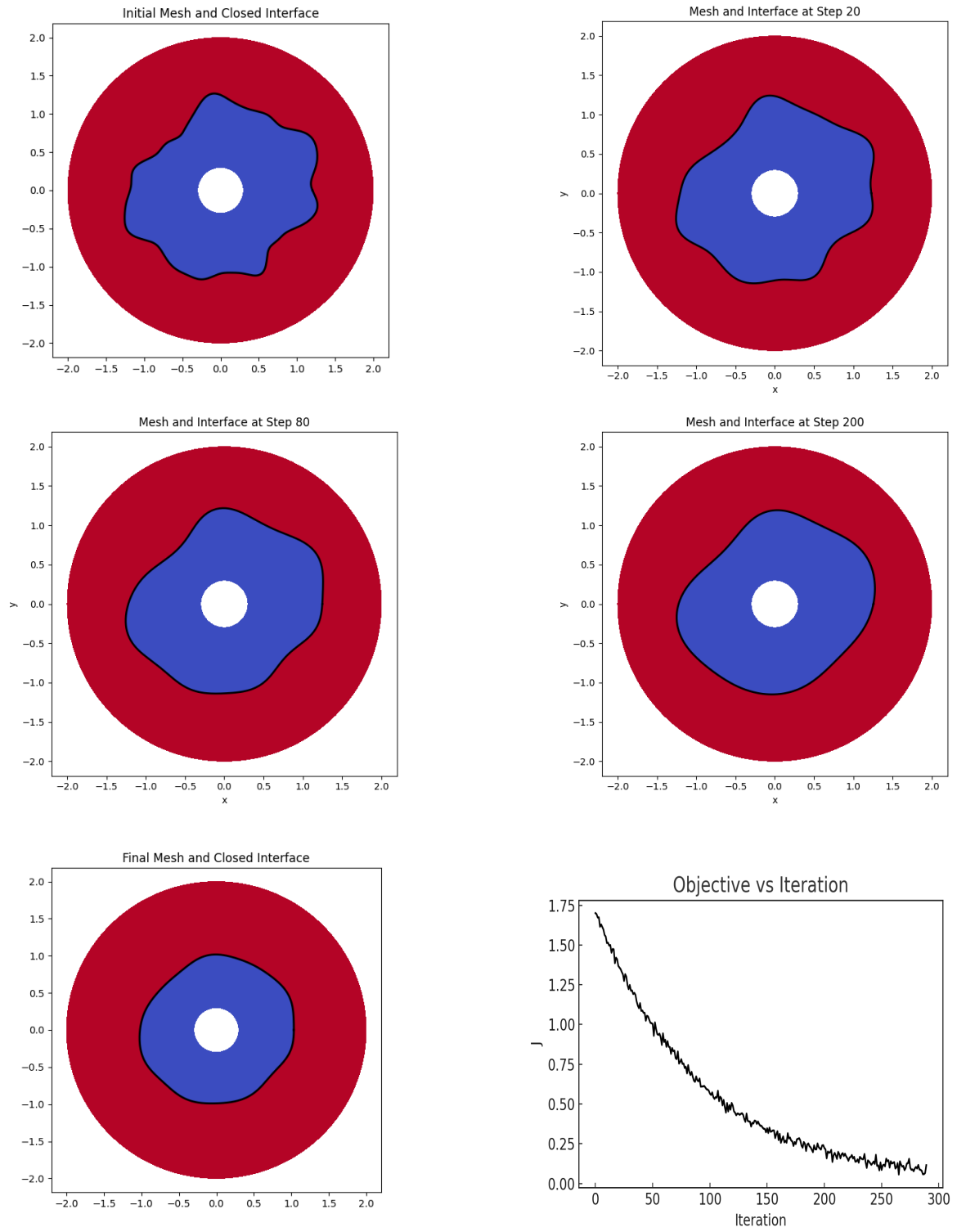


Figure 4.12: Evolution diagram when $\epsilon = 1 \times 10^{-2}$

Signorini-type contact conditions:

$$\left\{ \begin{array}{ll} -\operatorname{div}(\sigma(u)) = 0 & \text{in } D, \\ u = 0 & \text{on } \Gamma_3, \\ \llbracket u \rrbracket = 0, \quad \llbracket \sigma(u) \cdot n \rrbracket = 0 & \text{on } \Gamma \\ \sigma(u) \cdot n = P & \text{on } \Gamma_1, \\ \sigma(u) \cdot n = 0 & \text{on } \Gamma_2, \\ u \cdot n \leq 0, \quad \sigma(u) \cdot n \leq 0, \quad (u \cdot n)(\sigma(u) \cdot n) = 0 & \text{on } \Gamma_C. \end{array} \right. \quad (4.170)$$

Here, u is the displacement vector field, $\sigma(u) = \mathbb{C}\varepsilon(u)$ is the stress tensor, and $\varepsilon(u) = \frac{1}{2}(\nabla u + \nabla u^\top)$ is the linearized strain tensor. The material stiffness tensor $\mathbb{C}$ is assumed piecewise constant, reflecting different elastic properties on either side of an internal interface Γ separating subdomains.

The objective is to minimize the compliance functional:

$$J(\Gamma) = \frac{1}{2} \int_D \sigma(\psi) : \varepsilon(\psi), dx - \int_{\Gamma_1} P \cdot \psi, ds, \quad (4.171)$$

where ψ is the displacement field satisfying the elasticity system. Physically, $J(\Gamma)$ represents the total internal energy stored in the elastic system, adjusted for external work, and depends on the location and shape of Γ through the material tensor $\mathbb{C}$.

To regularize the evolution and ensure well-posedness, we augment the shape gradient dJ with a geometric regularization term $\mathcal{A}[f]$, typically derived from curvature-based energies such as elastica and perimeter:

$$\mathcal{A}[f] = \varepsilon_e \nabla_s^2 k + \frac{\varepsilon_e}{2} |k|^2 k - \varepsilon_p k, \quad (4.172)$$

where $k = \partial_s^2 f$ is the curvature vector, and ∇_s denotes the covariant derivative along the curve.

Combining the physical and geometric contributions, the full gradient flow is written as:

$$\left\{ \begin{array}{l} \partial_t f + \mathcal{A}[f] + \mathcal{B}[f] = 0, \\ f(0, \theta) = f_0(\theta), \end{array} \right. \quad (4.173)$$

where $\mathcal{B}[f] = dJ(f)$ denotes the Hadamard shape gradient of the compliance functional, and $\mathcal{A}[f]$ is the regularization gradient derived from intrinsic geometry.

This flow governs the evolution of the interface Γ in the direction of steepest descent of the total energy. The addition of curvature-based terms provides smoothing

and stabilizes the interface evolution against high-frequency instabilities, which are common in contact problems due to sharp stress transitions.

Figure 4.13 illustrates a typical configuration of the domain D , with labeled boundary segments and the evolving interface Γ .

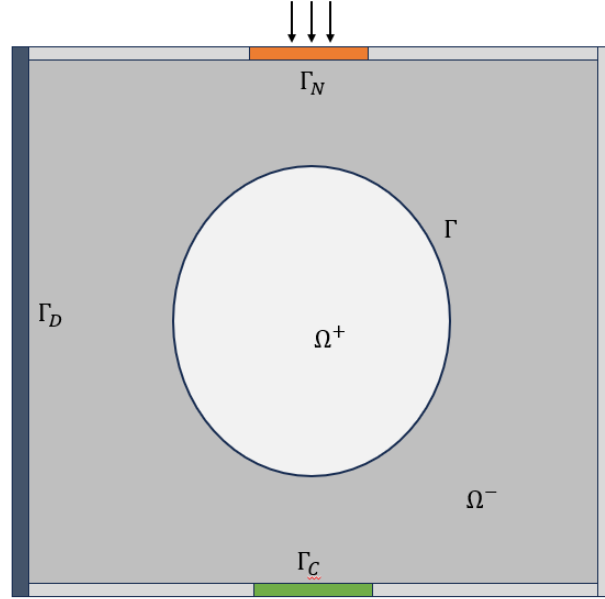


Figure 4.13: Elastic body with traction, clamped, and contact boundaries. The internal interface Γ separates regions with distinct material properties.

4.10.1 Shape sensitivity analysis of energy functional for unilateral contact problem

Even if the solution of variational inequality is only directionally shape differentiable, it turns out that the energy functional is shape differentiable. Therefore, we are able to write down the Gradient Flow system for the compliance minimization in $2D$ linear elasticity. The curve Γ divides the elastic body reference domain $\Omega = \Omega^+ \cup \Gamma \cup \Omega^-$ into two subdomains with two different material properties characterized by the fourth order Hooke's tensors $C^\pm$.

We consider the compliance minimization in Ω with the interface Γ . The cost functional is defined by minimization

$$J(\Gamma) = \inf_{v \in K} \left\{ \frac{1}{2} a(v, v) - L(v) \right\} = \left\{ \frac{1}{2} a(u, u) - L(u) \right\} \quad (4.174)$$

where

$$a(v, v) = \int_{\Omega^+} \sigma^+(v) : \varepsilon(v) + \int_{\Omega^-} \sigma^-(v) : \varepsilon(v) \quad (4.175)$$

and $L(v)$ corresponds to tractions P on Γ_1 . By $u \in K$ we denote the unique minimizer for the interface Γ .

When we move the interface according to the transformation $T_t(V) : \Omega \rightarrow \Omega$ we get $\Gamma_t = T_t(V)(\Gamma) = T_t(\Gamma)$. Then the elastic energy functional becomes

$$a_t(v \circ T_t^{-1}, v \circ T_t^{-1}) = \int_{\Omega_t^+} \sigma^+(v \circ T_t^{-1}) \varepsilon(v \circ T_t^{-1}) + \int_{\Omega_t^-} \sigma^-(v \circ T_t^{-1}) \varepsilon(v \circ T_t^{-1}) \quad (4.176)$$

and the shape functional

$$J(\Gamma_t) = \inf_{v \in K} \left\{ \frac{1}{2} a_t(v \circ T_t^{-1}, v \circ T_t^{-1}) - L(v \circ T_t^{-1}) \right\} = \frac{1}{2} a(u^t \circ T_t^{-1}, u^t \circ T_t^{-1}) - L(u^t \circ T_t^{-1}) \quad (4.177)$$

for the unique element $u^t \in K$.

In the Gradient Flow system we have the Hadamard shape gradient of

$$\Gamma \rightarrow J(\Gamma_t) \quad (4.178)$$

which is defined by the limit

$$\lim_{t \rightarrow 0} \frac{1}{t} (J(\Gamma_t) - J(\Gamma)). \quad (4.179)$$

To this end we differentiate the marginal function and we use the Hadamard structure Theorem of shape gradient of differentiable shape functional.

Lemma 4.10.1. *Let $v \in K \subset H^1(\Omega)$ be a fixed admissible function. Define the perturbed shape-dependent energy functional by*

$$j(t) := \frac{1}{2} a(v \circ T_t^{-1}, v \circ T_t^{-1}) - L(v), \quad (4.180)$$

where the transformation $T_t : \Omega \rightarrow \Omega_t$ is given by $T_t(x) = x + tV(x)$, with $V \in C^1(\bar{\Omega}; \mathbb{R}^n)$ a smooth vector field. Then the directional derivative at $t = 0^+$ is given by

$$j'(0^+) = \frac{1}{2} \int_{\Omega} \sigma(v) : \varepsilon(v) \operatorname{div} V + \int_{\Omega} \sigma(v) : \varepsilon'(v), \quad (4.181)$$

where $\varepsilon'(v)$ denotes the material derivative of the strain tensor under the shape perturbation.

Proof. To compute the shape derivative, we first note that the function $v \circ T_t^{-1}$ represents the pullback of v to the perturbed domain Ω_t . The energy functional becomes:

$$j(t) = \frac{1}{2} \int_{\Omega_t} \sigma(v \circ T_t^{-1}) : \varepsilon(v \circ T_t^{-1}) dx - L(v). \quad (4.182)$$

We pull back this integral to the reference domain Ω using the transformation $T_t(x) = x + tV(x)$. The Jacobian determinant of this transformation is:

$$\det(DT_t(x)) = 1 + t \operatorname{div} V(x) + o(t). \quad (4.183)$$

Substituting into the integral and differentiating with respect to t , we obtain:

$$\begin{aligned} j'(0^+) &= \frac{1}{2} \int_{\Omega} \sigma(v) : \varepsilon(v) \left. \frac{d}{dt} \det(DT_t(x)) \right|_{t=0} dx \\ &\quad + \int_{\Omega} \left. \frac{d}{dt} (\sigma(v \circ T_t^{-1}) : \varepsilon(v \circ T_t^{-1})) \right|_{t=0} dx \\ &= \frac{1}{2} \int_{\Omega} \sigma(v) : \varepsilon(v) \operatorname{div} V dx + \int_{\Omega} \sigma(v) : \varepsilon'(v) dx. \end{aligned} \quad (4.184)$$

The second term arises from differentiating the composition $\varepsilon(v \circ T_t^{-1})$, and the material derivative of the strain is given by:

$$\varepsilon'(v) = -\frac{1}{2} (Dv \cdot DV + DV^T \cdot Dv^T). \quad (4.185)$$

Since the load term $L(v)$ does not depend on t , its derivative vanishes. $\square$

We thus apply the result of the lemma. 4.10.1 to $v = u^t$, and deduce the shape derivative at $t = 0^+$, we will have the following result.

Lemma 4.10.2. *The shape functional is differentiable and its shape derivative takes the form*

$$dJ(\Gamma; V) = \frac{1}{2} \int_{\Omega} (\sigma(u) : \varepsilon(u)) (\operatorname{div} V) + \int \sigma(u) : \varepsilon'(u). \quad (4.186)$$

Remark 4.10.3. *In order to identify the boundary shape gradient on the interface we decompose integrals of the expression*

$$F(u, V) := \frac{1}{2} \sigma(u) : \varepsilon(u) (\operatorname{div} V) + \sigma(u) : \varepsilon'(u) \quad (4.187)$$

into two components

$$I = \int_{\Omega} F(u, V) = \int_{\Omega^+} F(u, V) + \int_{\Omega^-} F(u, V) = I^+ + I^- \quad (4.188)$$

and observe that by Stokes Theorem

$$\frac{1}{2} \int_{\Omega} \sigma(u) : \varepsilon(u) (\operatorname{div} V) = \frac{1}{2} \int_{\Gamma} \llbracket \sigma(u) : \varepsilon(u) \rrbracket v_n. \quad (4.189)$$

Therefore, we need only to provide the integration by parts Green's formula for the integrals

$$\int_{\Omega^+} \sigma(u) : \varepsilon'(u) + \int_{\Omega^-} \sigma(u) : \varepsilon'(u) := \int_{\Gamma} h(x) v_n(x) d\Gamma(x) \quad (4.190)$$

to obtain the Hadamard shape gradient

$$g(x)\mathbf{n} = \llbracket \sigma(u)(x) : \varepsilon(u)(x) \rrbracket \mathbf{n} + h(x)\mathbf{n} \quad (4.191)$$

for the Gradient Flow system of compliance minimization for unilateral contact problem in Ω .

The integration by parts formula is valid for the unique solution $u \in K$ of the contact problem which by the elliptic regularity is smooth on the both sides of Γ in an open neighbourhood $\mathcal{O}(\Gamma)$ of the interface Γ . We assume that the velocity field V is supported in the open set $\mathcal{O}(\Gamma) \subset \Omega$.

Next step is the identification of the Hadamard shape gradient which is given by a normal vector field on Γ . To this end we establish the Green formula for the second part of the shape derivative.

Since $V \mapsto dJ(\Gamma; V)$ is linear and continuous the structure theorem applies and we have

Lemma 4.10.4. *There is a distribution supported g on Γ such that*

$$dJ(\Gamma; V) = \langle g, v_n \rangle_{\{\mathcal{D}'_1(\Gamma), \mathcal{D}_1(\Gamma)\}}, \quad (4.192)$$

where v_n is the normal component of the vector field V .

For the vector field V we denote $V = v_n \mathbf{n} + v_\tau \tau$ the decomposition into normal and tangential components on Γ . Thus $V_i = v_n n_i + v_\tau \tau_i$ with $\mathbf{n} = (n_1, n_2)^\top$. We assume the regularity of the distribution $g \in L^1(\Gamma)$.

Let us consider $\int_{\Omega} \sigma(u) : \varepsilon'(u)$ where $\varepsilon'(u) = -\frac{1}{2} \{ Du DV + DV^\top DU^\top \}$. We have $(Du)_{ij} = u_{i,j}$ where $u_{i,j} = \frac{\partial u_i}{\partial x_j}$. We shall use the summation convention over repeated indices $i, j, k, l = 1, 2$.

We need the notation for two components of $\varepsilon'(u)$, namely for the expression

$$Du DV + DV^\top DU^\top = \sum_{j=1}^{j=2} \frac{\partial u_i}{\partial x_j} \frac{\partial DV_j}{\partial x_l} + \sum_{k=1}^{k=2} \frac{\partial u_k}{\partial x_i} \frac{\partial DV_l}{\partial x_k} = u_{i,j} DV_{j,l} + DV_{l,k} Du_{k,i}. \quad (4.193)$$

The classical Green's formula for two functions f, g in the domain Ω reads

$$\int_{\Omega} \frac{\partial f}{\partial x_i} g(x) dx = \int_{\Omega} f_{,i}(x) g(x) dx = - \int_{\Omega} g_{,i}(x) f(x) dx + \int_{\partial\Omega} f(x) g(x) n_i(x) d\Gamma(x), \quad (4.194)$$

where n_i stands for the component of exterior unit normal vector $\mathbf{n}$ on the boundary Γ . The same formula is applied on two subdomains $\Omega^{\pm}$.

We now expand the integrals involving the directional derivative of the strain tensor $\varepsilon'(u)$, which takes the form

$$\varepsilon'(u) = -\frac{1}{2} (\nabla u \cdot \nabla V + (\nabla V)^{\top} \cdot (\nabla u)^{\top}). \quad (4.195)$$

Consequently, the inner product with the stress tensor yields:

$$\sigma(u) : \varepsilon'(u) = -\frac{1}{2} (\sigma_{ik} u_{i,j} V_{j,k} + \sigma_{ik} u_{j,i} V_{k,j}), \quad (4.196)$$

where the summation convention over repeated indices is assumed.

We apply integration by parts separately on the two subdomains. For Ω^+ , we obtain:

$$\begin{aligned} \int_{\Omega^+} \sigma(u) : \varepsilon'(u) &= -\frac{1}{2} \int_{\Omega^+} (\sigma_{ik} u_{i,j} V_{j,k} + \sigma_{ik} u_{j,i} V_{k,j}) \\ &= \frac{1}{2} \int_{\Omega^+} (\partial_k (\sigma_{ik} u_{i,j}) + \partial_j (\sigma_{ik} u_{j,i})) V_j \\ &\quad - \frac{1}{2} \int_{\Gamma^+} (\sigma_{ik} u_{i,j} n_k + \sigma_{ik} u_{j,i} n_j) V_j. \end{aligned} \quad (4.197)$$

Similarly, for Ω^- , we derive:

$$\begin{aligned} \int_{\Omega^-} \sigma(u) : \varepsilon'(u) &= -\frac{1}{2} \int_{\Omega^-} (\sigma_{ik} u_{i,j} V_{j,k} + \sigma_{ik} u_{j,i} V_{k,j}) \\ &= \frac{1}{2} \int_{\Omega^-} (\partial_k (\sigma_{ik} u_{i,j}) + \partial_j (\sigma_{ik} u_{j,i})) V_j \\ &\quad + \frac{1}{2} \int_{\Gamma^-} (\sigma_{ik} u_{i,j} n_k + \sigma_{ik} u_{j,i} n_j) V_j. \end{aligned} \quad (4.198)$$

It is easy to check that the result for shape gradient obtained by replacement $V_i = v_n n_i + v_{\tau} \tau_i$ leads to the expression

$$\int_{\Gamma} h(x) v_n d\Gamma(x) = - \int_{\Gamma} \left[(\sigma(u) \mathbf{n}) \cdot \frac{\partial u}{\partial n} \right] v_n d\Gamma(x). \quad (4.199)$$

Lemma 4.10.5. *The shape gradient of the energy functional takes the form*

$$g(x) \mathbf{n} = \llbracket \sigma(u)(x) : \varepsilon(u)(x) \rrbracket \mathbf{n} - \left[\sigma(u)(x) \cdot \mathbf{n} \right] \cdot \frac{\partial u(x)}{\partial n} \mathbf{n} \quad (4.200)$$

$$dJ(\Gamma; V) = \int_{\Gamma} g(x) V \cdot \mathbf{n} \quad (4.201)$$

4.10.2 Numerical examples

Example 4.10.1. *In this example, we demonstrate the application of gradient flow-based shape optimization methods to the classic Signorini-type single-edge contact problem. The model is set up in a square computational domain $D = [0, 1]^2$, representing a linear elastic body under small deformation.*

The bottom center portion of the computational domain is designated as the potential contact region Γ_c , subject to frictionless Signorini-type constraints. Specifically, we impose a non-penetration condition in the normal direction and zero tangential stress. The top boundary uses a Neumann load condition: a vertical downward force is applied in the center cell to drive the deformation. The left boundary is fixed, i.e., we impose a uniform Dirichlet condition $u = 0$ on $\Gamma_D = \{0\} \times [0, 1]$. The remaining boundaries are frictionless.

The domain contains a material-pore interface represented by a smooth closed curve that evolves during the optimization process. This interface is described by Fourier parameterization:

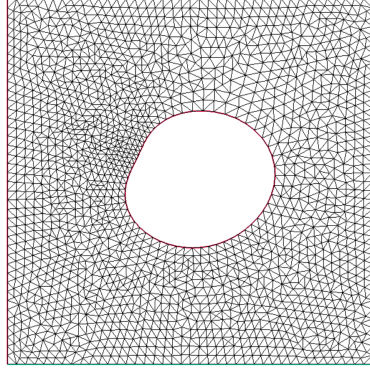
$$\Gamma_\varphi = \left\{ x(\theta) = x_0 + R(\theta) \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} : \theta \in [0, 2\pi) \right\}, \quad R(\theta) = \sum_{k=0}^N a_k \cos(k\theta) + b_k \sin(k\theta), \quad (4.202)$$

where $\{a_k, b_k\}$ are the Fourier coefficients encoding the shape. These coefficients constitute the shape variables and evolve via a gradient flow derived from the shape derivative of the compliance function under the Signorini constraint.

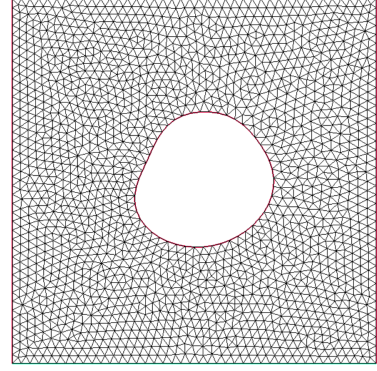
The objective function to be minimized is the compliance. The acceptable shape is implicitly represented by the Fourier-defined boundary.

The evolution of the interface follows the direction of steepest descent of $\mathcal{J}(\Omega)$ and is regularized by a Willmore-type curvature energy.

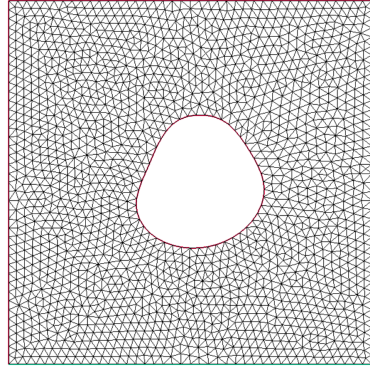
Figure 4.14 shows several snapshots of the interface evolution during the optimization process. The initial shape is a perturbed ellipse. As the iterations proceed, the interface gradually adapts to form a compliant structure that avoids contact violations while effectively transferring the applied loads. The objective function flattens out, indicating that the method converges. Figure 4.14f shows the evolution of the compliance value.



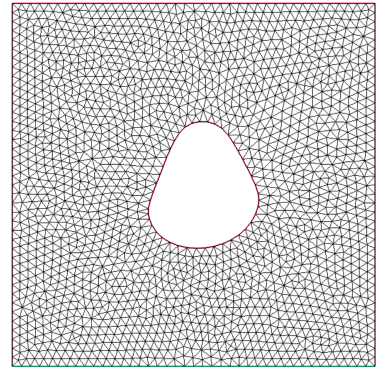
(a) Initial shape



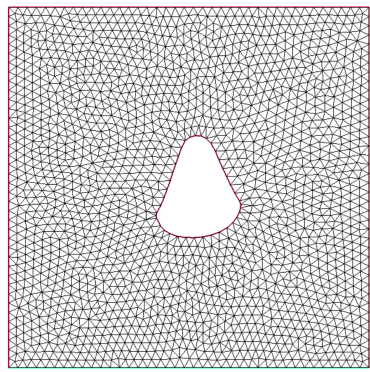
(b) Iteration 10



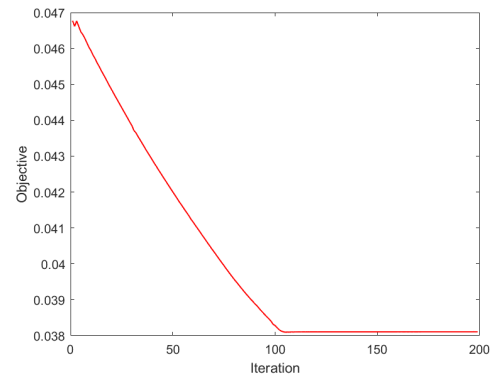
(c) Iteration 50



(d) Iteration 60



(e) Final design



(f) Objective function convergence

Figure 4.14: Gradient flow evolution under Signorini contact constraints for Example 4.10.1. Subfigures show the shape at selected iterations, and the objective value history.

Chapter 5

Structural Topology Optimization in Nonlinear Elasticity

In the previous chapters, we systematically explored the structural optimization and contact modeling problems based on linear elastic theory, including single-sided contact and friction boundary conditions in the phase field framework. The linear elastic model has good analytical and stability due to its linear mathematical structure and theoretical maturity. However, in many engineering applications and natural phenomena, material responses often show significant nonlinear characteristics Ganghoffer, Plotnikov, and Sokolowski, 2018, especially in large deformation, material constitutive nonlinearity Bendsøe, 2013 or geometric nonlinearity scenarios, where linear theory is no longer applicable.

Therefore, the following content will be extended to nonlinear elastic problems, aiming to study more general structural response behaviors. In this framework, shape optimization, variational principles and modeling will still be the core tools, but the mathematical structure of the problem must be reconstructed based on nonlinear strain energy functions and more complex state equations.

In the theory of nonlinear partial differential equations, it is a challenge to obtain new results on the existence of solutions to such models. We refer to the book published by Professor Demkowicz, in which he describes the latest progress in the field of approximation of nonlinear elastic mechanics.

Structural shape and topology optimization has been widely applied in industrial and engineering design, particularly for enhancing performance and structural stability. Classical approaches based on sensitivity analysis have been extensively developed; see, e.g., Bendsøe and Sigmund, 2004; Dapogny and Frey, 2010; Novotny et al., 2019a;

Sokolowski and Zolesio, 1992. In applications such as compliance minimization or compliant mechanism design Howell, 2001, the goal is to determine an optimal material distribution that ensures rigidity or flexibility under prescribed loading conditions while maintaining mechanical integrity.

Most existing models for structural topology optimization assume linear elasticity with small displacement gradients (cf. Jin et al., 2024; Nowak et al., 2020; Scheid and Sokolowski, 2018; Sokolowski and Tan, 2025). While this assumption is valid for a broad class of problems, it becomes inadequate in the presence of geometric or material nonlinearities, particularly under large deformations or complex load conditions. In such cases, nonlinear phenomena such as bending, buckling, and post-buckling responses significantly affect structural behavior and must be accounted for in both modeling and optimization.

To address these challenges, recent efforts have considered structural optimization under nonlinear elasticity. Among numerical discretization techniques, the discontinuous Galerkin finite element method (DGFEM) Tan and Zhu, 2023 has demonstrated significant advantages in solving partial differential equations, including elasticity problems. Unlike classical continuous finite element methods, DGFEM allows the use of element-wise polynomial approximations that are not required to be continuous across element interfaces. This flexibility facilitates the treatment of complex geometries, local adaptivity, and parallel implementations. The method employs weak formulations with numerical fluxes to handle inter-element discontinuities, which proves particularly beneficial in nonlinear and non-smooth problems.

Several studies have explored the integration of DGFEM into structural optimization. For instance, topology optimization with linear elasticity has been addressed using the SIMP method coupled with discontinuous Petrov–Galerkin formulations Evgrafov, 2018. In Adams et al., 2016, a level-set-based topology optimization framework was proposed, incorporating DGFEM with a symmetric interior penalty formulation Arnold et al., 2002 for spatial discretization of the elasticity equations and evolution of the level set function.

5.1 Nonlinear elasticity model

In nonlinear structural optimization, models incorporating hyperelastic materials are often employed. Let u denote the displacement field. The strain energy density is

defined as

$$W(E) = \frac{1}{2} E : A : E, \quad (5.1)$$

where E is the Lagrangian strain tensor and A is the fourth-order constitutive tensor for isotropic materials. The strain tensor E is given by

$$E = \frac{1}{2}(F^T F - I) = \frac{1}{2} (Du^T + Du + Du^T Du), \quad (5.2)$$

where $F = I + Du$ is the deformation gradient, and Du denotes the displacement gradient.

The constitutive tensor A for isotropic materials has the form

$$A = \lambda I \otimes I + 2\mu 1, \quad (5.3)$$

where λ and μ are the Lamé parameters, and the symmetric fourth-order identity tensor 1 is defined by $1_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$.

The second Piola–Kirchhoff stress tensor is then given by

$$T := \frac{\partial W}{\partial E} = A : E = \lambda \operatorname{tr}(E)I + 2\mu E. \quad (5.4)$$

Let $\Omega \subset \mathbb{R}^d$ denote the reference configuration of an elastic body, with boundary $\partial\Omega$ partitioned into three parts: Γ_D (Dirichlet boundary), Γ_N (Neumann boundary), and Γ (free boundary). The displacement field u satisfies the following boundary value problem:

$$\begin{cases} -\nabla \cdot T(u) = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ T(u)n = g & \text{on } \Gamma_N, \\ T(u)n = 0 & \text{on } \Gamma, \end{cases} \quad (5.5)$$

where f is the body force, g the applied surface traction, and n the outward unit normal vector.

The total potential energy of the nonlinear elastic system is defined as the difference between the stored strain energy and the work done by external forces:

$$\Pi(u) = \int_{\Omega} W(E) dx - \int_{\Omega} f \cdot u dx - \int_{\Gamma_N} g \cdot u ds. \quad (5.6)$$

The equilibrium configuration is obtained by minimizing the total potential energy. To derive the variational form, consider a perturbation $u_t = u + t\psi$, where $\psi \in \mathbf{V} := \{v \in H^1(\Omega)^d : v = 0 \text{ on } \Gamma_D\}$. Then the first variation of the potential energy at $t = 0$ is

$$\left. \frac{d}{dt} \Pi(u_t) \right|_{t=0} = \int_{\Omega} T(u) : \hat{E}(u, \psi) dx - \int_{\Omega} f \cdot \psi dx - \int_{\Gamma_N} g \cdot \psi ds, \quad (5.7)$$

where

$$\hat{E}(u, \psi) = \left. \frac{d}{dt} E(u_t) \right|_{t=0} = \frac{1}{2} (F^T D\psi + D\psi^T F) = \mathcal{S}(FD\psi), \quad (5.8)$$

and $\mathcal{S}(M) := \frac{1}{2}(M + M^T)$ denotes the symmetric part of a matrix M .

Thus, the weak form of the nonlinear elasticity problem is: find $u \in \mathbf{V}$ such that

$$a(u, \psi) = l(\psi), \quad \forall \psi \in \mathbf{V}, \quad (5.9)$$

with bilinear and linear forms defined by

$$a(u, \psi) := \int_{\Omega} A : E(u) : \hat{E}(u, \psi) dx, \quad l(\psi) := \int_{\Omega} f \cdot \psi dx + \int_{\Gamma_N} g \cdot \psi ds. \quad (5.10)$$

For structural topology optimization, we consider the minimization problem

$$\min_{\Omega} \{J(\Omega) := -\Pi(u) + \ell \cdot \text{Vol}(\Omega)\}, \quad (5.11)$$

where $\ell > 0$ is a fixed Lagrange multiplier imposing a volume constraint.

5.2 Shape sensitivity analysis

Shape sensitivity analysis based on shape calculus is a valuable tool for designing numerical methods for shape optimization. We use the perturbation of identity method, which is equivalent to the velocity method and method of mapping in the sense of first-order Taylor expansion. For $t \in [0, \varepsilon_1)$ ($\varepsilon_1 > 0$), define a family of smooth mappings $\{F_t\}_{t \in [0, \varepsilon_1)}$ with $F_t : \bar{D} \rightarrow \bar{D}$. The boundary Γ_D is fixed, i.e., $F_t(\Gamma_D) = \Gamma_D$. Then we denote $\Omega_t := F_t(\Omega) = \{F_t(x) : x \in \Omega\}$ with $\Omega_0 = \Omega$ and the boundary $\partial\Omega_t := F_t(\partial\Omega) = \{F_t(x) : x \in \partial\Omega\}$ with $\partial\Omega_0 = \partial\Omega$. The mappings $\{F_t\}_{t \in [0, \varepsilon_1)}$ describe the motion of each point in D , i.e., at $t \in [0, \varepsilon_1]$, the point $x \in D$ has a new position $x_t := F_t(x) \in D$ with $x_0 = x$. More specifically,

$$F_t = \text{Id} + t\theta,$$

where Id represents the identity mapping and $\theta = \theta(x)$ denotes a sufficiently smooth vector field in

$$\Theta_{ad} = \{\theta \in W^{1,\infty}(D; \mathbb{R}^d) \mid \theta = 0 \text{ on } \Gamma_D\}. \quad (5.12)$$

Here, $W^{1,\infty}(D; \mathbb{R}^d)$ is the space of vector field functions for which each of its components belongs to $W^{1,\infty}(D)$, a Banach space of functions uniformly bounded up to first-order weak derivative.

For shape perturbations of the field variable, let u and u_t be two state fields related to domains Ω and Ω_t , respectively. We defined the considered shapes belong the admissible set

$$\mathcal{U}_{ad} := \{\Omega \subset D \text{ is bounded and Lipschitz}\}.$$

Definition 5.2.1. For a real-valued shape functional $J : \Omega \mapsto \mathbb{R}$, A shape functional J is called shape differentiable at Ω , if

$$dJ(\Omega; \theta) := \lim_{t \searrow 0} \frac{J(\Omega_t) - J(\Omega)}{t} \quad (5.13)$$

exists for all directions θ and the mapping $\theta \mapsto dJ(\Omega; \theta)$ is linear and continuous. The expression $dJ(\Omega; \theta)$ is called as an Eulerian derivative of J at Ω in direction θ .

Lemma 5.2.2. Let Ω be a smooth bounded open set. Then for

$$J(\Omega) = \int_{\Omega} f dx \quad (5.14)$$

with $f = f(x) \in W^{1,1}(\mathbb{R}^d)$, J is differentiable at Ω and for any $\theta \in W^{1,\infty}(D; \mathbb{R}^d)$

$$dJ(\Omega; \theta) = \int_{\Omega} (\dot{f} + f \operatorname{div} \theta) dx, \quad (5.15)$$

in which $\dot{f} = \nabla f \cdot \theta$. If, in addition, Ω is of class C^1 , it holds that

$$dJ(\Omega; \theta) = \int_{\partial\Omega} f \theta_n ds, \quad (5.16)$$

where $\theta_n = \theta \cdot n$.

For shape sensitivity analysis of nonlinear elasticity, consider an objective

$$J(u) = \int_{\Omega} j(u) dx + \int_{\Gamma_N} l(u) ds, \quad (5.17)$$

where $j(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}$ and $l(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}$ are C^1 . We denote Tan et al., 2024

$$\delta T = \frac{\partial T}{\partial E} : \delta E = A : \delta E, \quad (5.18)$$

where δT is the stress variation and δE is the strain variation. By noting that the increment of deformation gradient is $\delta F = D\delta u$. Then, the increment of the Lagrangian strain and its variation can be obtained respectively as

$$\delta E(u, \delta u) = \mathcal{S}(F \cdot D\delta u), \quad \delta \hat{E}(\delta u, \psi) = \mathcal{S}(D\delta u \cdot D\psi). \quad (5.19)$$

Introduce a Lagrangian with $v, q \in \mathbf{V}$

$$\begin{aligned} \mathcal{L}(\Omega, v, q) = & \int_{\Omega} j(v) \, dx + \int_{\Gamma_N} l(v) \, ds + \int_{\Omega} A : E(v) : \hat{E}(v, q) \, dx \\ & - \int_{\Omega} f \cdot q \, dx - \int_{\Gamma_N} g \cdot q \, ds. \end{aligned} \quad (5.20)$$

The first-order optimality condition implies for $\mathcal{L}$ at (u, p) in the direction $\psi \in \mathbf{V}$ that

$$\begin{aligned} 0 = & \left\langle \frac{\partial}{\partial v} \mathcal{L}(\Omega, u, p), \psi \right\rangle \\ = & \int_{\Omega} j'(u) \cdot \psi \, dx + \int_{\Gamma_N} l'(u) \cdot \psi \, ds + \int_{\Omega} (\delta T(u) \psi : \hat{E}(u, p) + T(u) : \delta \hat{E}(u, p) \psi) \, dx \\ = & \int_{\Omega} j'(u) \cdot \psi \, dx + \int_{\Gamma_N} l'(u) \cdot \psi \, ds + \int_{\Omega} (A : \delta \tilde{E}(u, \psi) : \hat{E}(u, p) + T(u) : \delta \bar{E}(u, p, \psi)) \, dx, \end{aligned} \quad (5.21)$$

where we denote $\delta \tilde{E}(u, \psi) := \delta E(u) \psi$ and $\delta \bar{E}(u, p, \psi) := \delta \hat{E}(u, p) \psi$. Therefore, the weak form of adjoint reads as

$$\int_{\Omega} (A : \delta \tilde{E}(u, \psi) : \hat{E}(u, p) + T(u) : \delta \bar{E}(u, p, \psi)) \, dx = - \int_{\Omega} j'(u) \cdot \psi \, dx - \int_{\Gamma_N} l'(u) \cdot \psi \, ds, \quad (5.22)$$

where $T = A : E$. Define

$$\mathbf{V}_t := \{v \in H^1(\Omega_t) : v = 0 \text{ on } \Gamma_D\}. \quad (5.23)$$

Theorem 5.2.3 (Compliance in nonlinear elasticity). *Let Ω be an open bounded domain. Let u and p be weak solutions to (5.9) and (5.22) in nonlinear elasticity, respectively. Then, the distributed Eulerian derivative of (5.17) reads:*

$$\begin{aligned} dJ(\Omega; \theta) = & \int_{\Omega} \left(A \partial_t \mathcal{E}(0, u) : \mathcal{E}(0, u, p) + A \mathcal{E}(0, u) : \partial_t \mathcal{E}(0, u, p) \right. \\ & \left. + A \mathcal{E}(0, u) : \mathcal{E}(0, u, p) \operatorname{div} \theta + \operatorname{div}(j(u) \theta) - \operatorname{div}(f \cdot p \theta) \right) \, dx, \end{aligned} \quad (5.24)$$

where

$$\partial_t \mathcal{E}(0, u) = -\mathcal{S}(\operatorname{Du} \operatorname{D} \theta) - \mathcal{S}(\operatorname{D} \theta^T \operatorname{Du}^T \operatorname{Du}), \quad (5.25)$$

$$\partial_t \mathcal{E}(0, u, p) = -\mathcal{S}(\operatorname{D} p \operatorname{D} \theta) - \mathcal{S}(\operatorname{D} \theta^T \operatorname{Du}^T \operatorname{D} p) - \mathcal{S}(\operatorname{Du}^T \operatorname{D} p \operatorname{D} \theta), \quad (5.26)$$

$$\mathcal{E}(0, u) = \mathcal{S}(\operatorname{Du}) + \frac{1}{2} \operatorname{Du}^T \operatorname{Du}, \quad (5.27)$$

$$\mathcal{E}(0, u, v) = \mathcal{S}(\operatorname{D} v + \operatorname{D} v^T \operatorname{Du}). \quad (5.28)$$

If, moreover, Ω is sufficiently smooth, $J(\Omega)$ is shape differentiable and its boundary type of Eulerian derivative reads:

$$dJ(\Omega; \theta) = \int_{\Gamma} (j(u) + A : E(u) : \hat{E}(u, p) - f \cdot p + \ell) \theta_n \, ds, \quad (5.29)$$

where $\theta_n = \theta \cdot n$.

Proof. We minimize the cost functional (5.17).

The variational form of nonlinear elasticity is to find $u \in \mathbf{V}$ such that

$$\int_{\Omega} A : E(u) : \hat{E}(u, v) \, dx = \int_{\Omega} f \cdot v \, dx + \int_{\Gamma_N} g \cdot v \, ds \quad \forall v \in \mathbf{V}. \quad (5.30)$$

Denote by u_t the solution of nonlinear elasticity system with Ω replaced by Ω_t . Let $u^t = u_t \circ T_t$ and use the chain rule to have

$$Du^t = D(u_t \circ T_t) = (Du_t) \circ T_t DT_t. \quad (5.31)$$

Consequently,

$$\begin{aligned} \mathcal{E}(t, u^t) &:= E(u_t) \circ T_t = \frac{1}{2} (Du_t + Du_t^T + Du_t^T Du_t) \circ T_t \\ &= \mathcal{S}(Du^t DT_t^{-1}) + [(DT_t)^{-T} (Du^t)^T] [Du^t (DT_t)^{-1}] / 2. \end{aligned} \quad (5.32)$$

and

$$\begin{aligned} \mathcal{E}(t, u^t, v^t) &:= \hat{E}(u_t, v_t) \circ T_t = \frac{1}{2} (Dv_t + Dv_t^T + Dv_t^T Du_t + Du_t^T Dv_t) \circ T_t \\ &= \mathcal{S}(Dv^t DT_t^{-1}) + \mathcal{S}([(DT_t)^{-T} (Du^t)^T] [Dv^t (DT_t)^{-1}]). \end{aligned} \quad (5.33)$$

The variational formulation for state on Ω_t is to find $u_t \in \mathbf{V}_t$ such that

$$\int_{\Omega_t} A_{\Omega_t} : E(u_t) : \hat{E}(u_t, v_t) \, dx_t = \int_{\Omega_t} f \cdot v_t \, dx_t + \int_{\Gamma_N} g \cdot v_t \, ds_t \quad \forall v_t \in \mathbf{V}_t. \quad (5.34)$$

Denote by $\xi(t) := \det DT_t$ the determinant of the Jacobian of transformation. Note that neither the Jacobian nor T_t needs to appear in the integrals on Γ_N and Γ , since we have assumed $T_t = \text{Id}$ on $\Gamma_D \cup \Gamma_N \cup \Gamma$. In view of (5.33), taking $v_t = v \circ T_t^{-1}$ for any $v \in \mathbf{V}$ in (5.34), we can have

$$\begin{aligned} \int_{\Omega} A_{\Omega} : \mathcal{E}(t, u^t) : \mathcal{E}(t, u^t, v) \xi(t) \, dx &= \int_{\Omega} (f \circ T_t) \cdot v \xi(t) \, dx \\ &\quad + \int_{\Gamma_N} (g \circ T_t) \cdot v \xi(t) |DT_t^{-T} n| \, ds \quad \forall v \in \mathbf{V}. \end{aligned} \quad (5.35)$$

For shape functional,

$$\begin{aligned} J(\Omega_t) &= \int_{\Omega_t} j(u_t) dx_t + \int_{\Gamma_N} l(u_t) ds_t \\ &= \int_{\Omega} j(t, u^t) \xi(t) dx + \int_{\Gamma_N} l(t, u^t) \xi(t) |DT_t^{-T} n| ds, \end{aligned} \quad (5.36)$$

where we denote $j(t, u^t) := j(u_t \circ T_t)$ and $l(t, u^t) := l(u_t \circ T_t)$. Introduce a Lagrangian

$$\begin{aligned} L(t, \varphi, \psi) &:= \int_{\Omega} j(t, \varphi) \xi(t) dx + \int_{\Gamma_N} l(t, \varphi) \xi(t) |DT_t^{-T} n| ds \\ &+ \int_{\Omega} A_{\Omega} \mathcal{E}(t, \varphi) : \mathcal{E}(t, \varphi, \psi) \xi(t) dx - \int_{\Omega} (f \circ T_t) \cdot \psi \xi(t) dx - \int_{\Gamma_N} (g \circ T_t) \cdot \psi \xi(t) |DT_t^{-T} n| ds. \end{aligned} \quad (5.37)$$

In view of (5.35) and (5.36), we have $J(\Omega_t) = L(t, u^t, \psi)$ for all $\psi \in \mathbf{V}$. Thus the shape derivative can be computed as

$$dJ(\Omega; \theta) = \left. \frac{d}{dt} L(t, u^t, \psi) \right|_{t=0}. \quad (5.38)$$

The advantage of the Lagrangian is that, under suitable assumptions, one can show that

$$\left. \frac{d}{dt} L(t, u^t, \psi) \right|_{t=0} = \partial_t L(0, u^0, p^0), \quad (5.39)$$

which essentially means that it is unnecessary to compute the derivative of u^t to compute $dJ(\Omega; \theta)$.

Using (5.38) and (5.39), we obtain (5.24).

To derive the boundary form of the Eulerian derivative, consider a Lagrangian

$$\mathcal{L}(\Omega, u, p) = \int_{\Omega} j(u) dx + \int_{\Omega} A : E(u) : \hat{E}(u, p) dx - \int_{\Omega} f \cdot p dx - \int_{\Gamma_N} g \cdot p ds + \ell \text{Vol}(\Omega). \quad (5.40)$$

We have

$$\begin{aligned} dJ(\Omega; \theta) &= \int_{\partial\Omega} (j(u) + A : E(u) : \hat{E}(u, p) - f \cdot p + \ell) \theta_n ds \\ &\quad - \int_{\Gamma_N} \left(\frac{\partial(g \cdot p)}{\partial n} + \kappa(g \cdot p) \right) \theta_n ds, \end{aligned} \quad (5.41)$$

where κ is the mean curvature. Since the boundary Γ_N and Γ_D are not deformed, we obtain the boundary expression (5.29). $\square$

5.3 Discontinuous Galerkin finite element method

Level set method Osher and Sethian, 1988 as a general implicit interface-tracking technique for computation of evolving interfaces using an implicit representation of these interfaces has been successfully applied in shape and topology optimization (see, e.g., Béatrice Rivière and Whiteman, 2003; Grégoire Allaire, 2021; Hansbo and Larson, 2022). The method represents the boundary of the moving domain $\Omega_t \subset D \subset \mathbb{R}^d$ as the zero level set of a continuous function $\phi(t, \cdot) : D \rightarrow \mathbb{R}$. Each domain Ω_t can be represented as

$$\Omega_t := \{x \in D | \phi(t, x) < 0\}, \quad (5.42)$$

where $\phi : \mathbb{R}^+ \times D \rightarrow \mathbb{R}$ is a Lipschitz continuous level set function. The boundary $\partial\Omega_t$ can be the zero level set of $\phi(t, \cdot)$:

$$\partial\Omega_t = \{x \in D | \phi(t, x) = 0\}. \quad (5.43)$$

Let $x(t)$ be the position of a moving boundary point of $\partial\Omega_t$, with velocity $\dot{x}(t) = \theta(x(t))$. Differentiating the relation $\phi(x(t), t) = 0$ with respect to t yields

$$\phi_t(t, x(t)) + \theta(x(t)) \cdot \nabla \phi(t, x(t)) = 0 \quad \text{in } \partial\mathbb{R}^+ \times \Omega_t, \quad (5.44)$$

which is then extended to $\mathcal{D}$ to obtain a transport equation

$$\phi_t(t, x) + \theta(x) \cdot \nabla \phi(t, x) = 0 \quad \text{in } \mathbb{R}^+ \times D. \quad (5.45)$$

Rewrite (5.45) as $\mathcal{A}\phi(t, x) = 0$, where

$$\mathcal{A}\phi = \phi_t(t, x) + \theta(t, x) \cdot \nabla \phi(t, x).$$

We use DGFEM for spatial discretizations of the transport equation of level set function (see Tan and Zhu, 2023). Consider a two-dimensional case for simplicity. Let $\{\mathcal{I}_h\}_{h>0}$ be a family of triangular meshes of D . Denote by P_{1dc} the space of piecewise linear break element polynomials. Define

$$\begin{aligned} W &= \{v \in L^2(D) | \theta \cdot \nabla v \in L^2(D)\}, \\ W_h &= \{v_h \in L^2(D) | \forall K \in \mathcal{I}_h, v_h|_K \in \mathbb{P}^1(K)\}. \end{aligned}$$

Let $W(h) = H^1(D) + W_h$. To enforce boundary conditions, define

$$\partial D^\pm = \{x \in \partial D | \pm \theta(x) \cdot n(x) > 0\} \quad (5.46)$$

and assume that ∂D^- and ∂D^+ are well-separated.

Denote by $\mathcal{F}_h$ the set of interior faces, i.e., $F \in \mathcal{F}_h$ if F is a 1-manifold and there are $K_1(F), K_2(F) \in \mathcal{I}_h$ such that $F = K_1(F) \cap K_2(F)$. Moreover, denote by $\mathcal{F}_h^\partial$ the set of the faces that separate the mesh from the exterior of D , i.e., $F \in \mathcal{F}_h^\partial$ if F is a 1-manifold and there is $K(F) \in \mathcal{I}_h$ such that $F = K(F) \cap \partial D$. Finally, we set $\mathcal{F}_h = \mathcal{F}_h \cup \mathcal{F}_h^\partial$.

We introduce $\mathcal{D}$ and $\mathcal{M} : \partial D \rightarrow \mathbb{R}$ which has the following representation: for all functions $v, w \in W$

$$\begin{aligned} \langle \mathcal{D}v, w \rangle_{W', W} &= \int_{\partial D} vw(\theta \cdot n) ds \\ \langle \mathcal{M}v, w \rangle_{W', W} &= \int_{\partial D} vw|\theta \cdot n| ds. \end{aligned} \quad (5.47)$$

For any measurable subset of D , let $(\cdot, \cdot)_{L, E}$ denotes the usual L^2 scalar product on E . Thus we define the bilinear form

$$\tilde{a}(\phi, w) = (\mathcal{A}\phi, w)_L + \frac{1}{2} \langle (\mathcal{M} - \mathcal{D})\phi, w \rangle_{W', W}. \quad (5.48)$$

To control the jumps of functions in W_h across mesh interfaces, we introduce for all $F \in \mathcal{F}_h$ a linear operator $S_F \in \mathcal{L}(L^2(F); L^2(F))$

$$S_F = \alpha|\theta \cdot n_F|, \quad (5.49)$$

where n_F is a unit normal vector to F . Since every function v in $W(h)$ has a (possibly two-valued) trace almost everywhere on $F \in \mathcal{F}_h$, it means that for a.e. $x \in F$,

$$v^1(x) = \lim_{\substack{y \rightarrow x \\ y \in K_1(F)}} v(y), \quad v^2(x) = \lim_{\substack{y \rightarrow x \\ y \in K_2(F)}} v(y). \quad (5.50)$$

Thus, we denote on F

$$[[v]] = v^1 - v^2, \quad \{v\} = \frac{1}{2}(v^1 + v^2).$$

Introduce the bilinear form $\tilde{a}_h$ such that for all ϕ, w in $W(h)$,

$$\begin{aligned} \tilde{a}_h(\phi, w) &= \sum_{K \in \mathcal{I}_h} (\mathcal{A}\phi, w)_{L, K} + \sum_{K \in \mathcal{F}_h^\partial} \frac{1}{2} (\mathcal{M}(\phi) - \mathcal{D}\phi, w)_{L, F} \\ &\quad - \sum_{K \in \mathcal{F}_h} 2(\{\mathcal{D}\phi\}, \{w\})_{L, F} + \sum_{F \in \mathcal{F}_h} (S_F([[\phi]]), [[w]])_{L, F}. \end{aligned} \quad (5.51)$$

The element flux of a function v on ∂K , say $\zeta_{\partial K}(v) \in L^2(\partial K)$, is defined on a face $F \subset \partial K$ by

$$\zeta_{\partial K}(v)|_F = \begin{cases} \frac{1}{2}\mathcal{M}(v|_F) - \frac{1}{2}\mathcal{D}v & \text{if } F \in \mathcal{F}^\partial \\ S_F([[v]]_{\partial K}|_F) - \mathcal{D}\{v\}_{\partial K} & \text{if } F \in \mathcal{F}. \end{cases}$$

Then we have the discretized variational formulation: Find $\phi_h \in W_h$ such that $\forall K \in \mathcal{T}_h$

$$(\mathcal{A}\phi_h, w_h)_{L,K} + (\zeta_{\partial K}(\phi_h), w_h)_{L,\partial K} = 0, \quad w_h \in W_h \quad (5.52)$$

Here, the interface/boundary flux of the level-set transport equation is

$$\zeta_{\partial K}(\phi_h)|_F = \begin{cases} (\alpha|\theta \cdot n_K| - \frac{1}{2}\theta \cdot n_K) \llbracket \phi_h \rrbracket_{\partial K} & \text{if } F \in \mathcal{F}^\partial \\ -|\theta \cdot n| \phi_h 1_{\partial D^-} & \text{if } F \in \mathcal{F}, \end{cases}$$

where $1_{\partial D^-}$ denotes the characteristic function of ∂D^- . We now consider time discretization using the backward Euler method. Denote by $\delta t > 0$ the time step. Let ϕ_h^n be an approximation to $\phi^n = \phi(t_n, x)$ at $t_n = n\delta t$. The space-time discretization of (5.52) reads: Given ϕ_h^n ($n = 0, 1, \dots$), find $\phi_h^{n+1} \in W_h$ such that $\forall w \in W_h$

$$\begin{aligned} \int_D \left(\frac{\phi_h^{n+1} - \phi_h^n}{\delta t} + \theta \cdot \nabla \phi_h^{n+1} \right) w dx + \sum_{\partial K} \int_{\partial K} \left(\alpha |n_K \cdot \theta| - \frac{1}{2} n_K \cdot \theta \right) \llbracket \phi_h^{n+1} \rrbracket w ds \\ - \sum_{\partial K_\Gamma^-} \int_{K_\Gamma^-} |n \cdot \theta| \phi_h^{n+1} w ds = 0, \end{aligned} \quad (5.53)$$

where ∂K is the set of inner edges and ∂K_Γ^- is the set of boundary edges where $\theta \cdot n_K < 0$. The normal vector n_K here is the normal to the edges of each inner element.

For reinitialization of the level set function, we use an effective iteration scheme integrated into FreeFem++ as a plug-in function *distance* to complete periodical reinitialization Dapogny and Frey, 2010.

5.4 Numerical examples

Example 5.4.1 (Nonlinear elasticity: cantilever beam design). *To investigate the effect of geometric nonlinearity on structural optimization, we consider the classical cantilever beam problem under nonlinear elastic conditions. The goal is to maximize the structural stiffness, which corresponds to minimizing the compliance subject to volume constraints.*

The computational domain, boundary conditions, and loads are the same as for the linear elastic cantilever beam problem (see Figure 5.1, top left). Specifically, the left edge of the rectangular domain is fixed (Dirichlet condition) and a downward vertical load is applied at the midpoint of the right edge (Neumann condition). The structure is initially filled with material, and void regions are iteratively introduced during the optimization process.

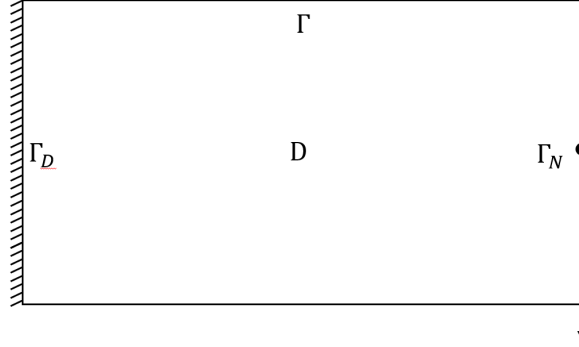


Figure 5.1: Model setup

We consider hyperelastic material behavior, whose energy density and stress-strain relations are described in the nonlinear elasticity section. The optimization is performed using shape derivatives derived from the nonlinear system, and the domain evolution is controlled by gradient descent with regularization. The volume constraint is enforced by a Lagrange multiplier with parameter $\ell = 15$. We use level sets to track the evolution of the domain, and the level set evolution equations are solved using the discontinuous Galerkin finite element method.

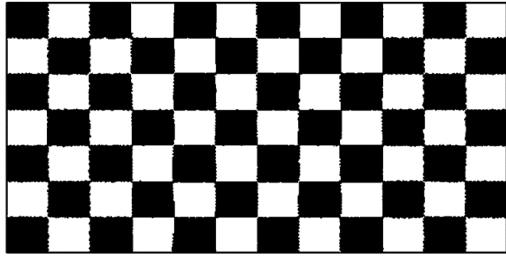
Figure 5.2 shows the evolution of the domain from an initial guess (top left) to the optimized design (bottom right). This is due to the greater flexibility and redistribution of stress paths allowed by the geometric nonlinearity.

Figure 5.3 quantitatively demonstrates the convergence behavior, where we show how the objective function and volume fraction evolve during the iterations. The plot confirms the stable convergence of the optimization process and illustrates how the final design effectively utilizes the available volume to enhance stiffness under large deformation effects.

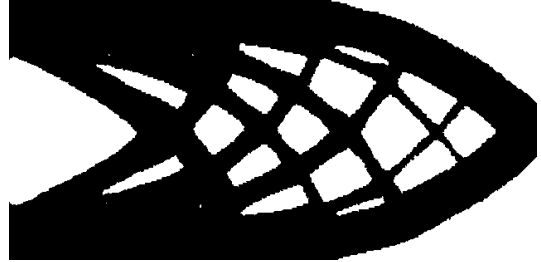
This example highlights the importance of considering nonlinear effects in topology and shape optimization, especially when large displacements or geometric instabilities are involved.

Example 5.4.2 (Nonlinear elasticity: MBB beam). This example considers the structural optimization of an MBB beam under nonlinear elasticity, aiming to minimize the compliance while maintaining a volume constraint. The geometry and mesh are the same as in Figure 5.4a (left), except for the boundary conditions applied in the lower right corner. Specifically, Dirichlet boundary conditions are applied at both ends of the bottom edge, and Neumann loads are applied on the rest.

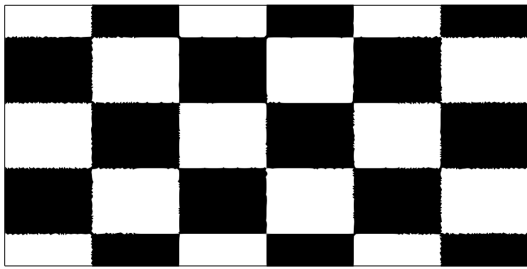
The regularization parameter is set to $\ell = 10$, and the optimization is performed



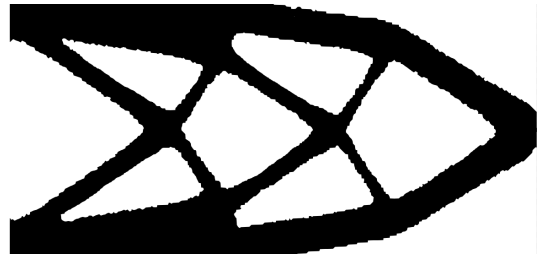
(a) Complicated initial design



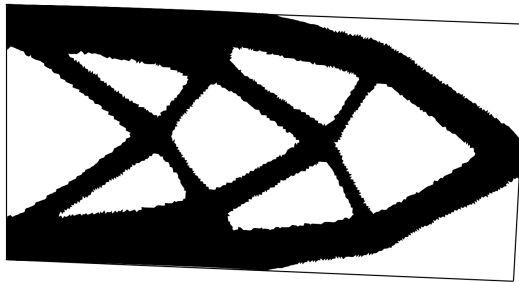
(b) Final design (from complicated)



(c) Simple initial design

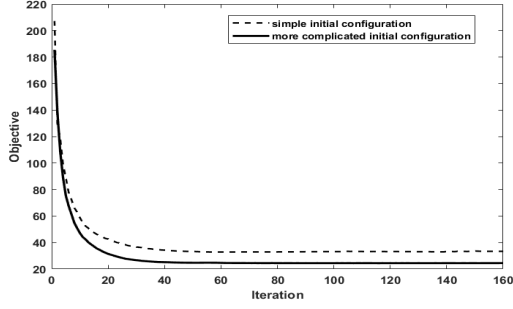


(d) Final design (from simple)

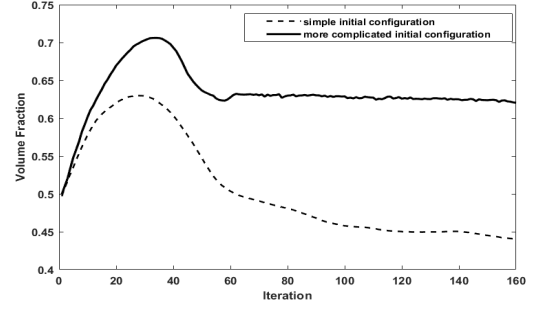


(e) Deformed final structure

Figure 5.2: Optimization results for Example 5.4.1. Top row: evolution from a complex initial guess to an optimized shape. Bottom row: evolution from a simpler initial guess and corresponding deformed structure under load.



(a) Objective value convergence



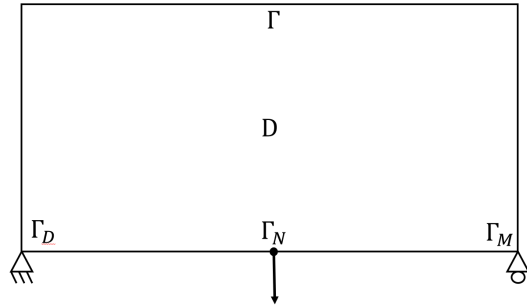
(b) Volume fraction history

Figure 5.3: Convergence history of objective (left) and volume fraction (right) of Example 5.4.1.

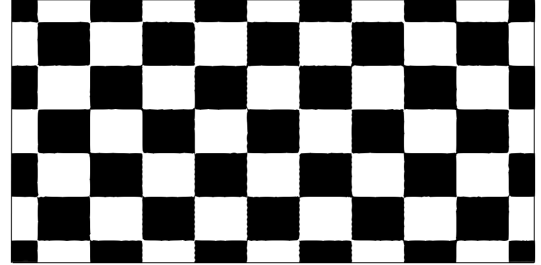
using the nonlinear hyperelastic material law as described in Section X.X. The goal is to evolve the structure to an optimal material distribution that provides maximum stiffness under a given load.

We employ the level set method to implicitly represent the shape and its evolution over time. To solve the level set evolution equations efficiently and accurately, we use the discontinuous Galerkin finite element method (DGFEM) due to its advantages in handling hyperbolic equations with discontinuities and its compatibility with unstructured meshes and local adaptivity. The DG scheme enables a stable and high-order accurate approximation of the level set transport equations, especially in cases with sharp topological transitions and interface evolution.

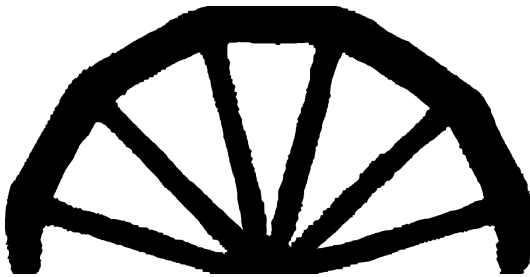
Figure 5.4 shows the initial configuration, the optimized material distribution, and the deformed shape under applied load, highlighting the effect of nonlinear elasticity. The convergence history of the objective function (compliance) is shown in Figure 5.5, demonstrating the effectiveness of the optimization process. The final design has clear load paths and structurally efficient material configurations, demonstrating the potential of combining nonlinear material models with a level set-based shape optimization framework.



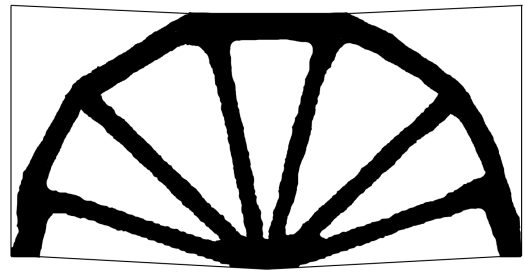
(a) Design domain



(b) Initial shape

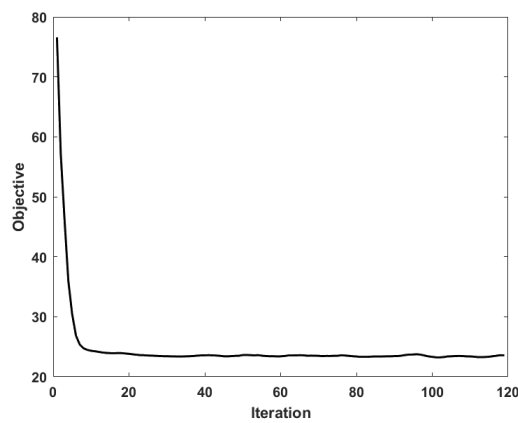


(c) Final design



(d) Deformed structure

Figure 5.4: Shape evolution in nonlinear elasticity for Example 5.4.2: (a) design domain, (b) initial guess, (c) optimized structure, (d) deformed shape under load.



(a) Objective value vs. iteration

Figure 5.5: Convergence history of the objective function for Example 5.4.2.

Conclusion

Conclusion

This thesis presents a comprehensive study of optimal design problems in elasticity with boundary control and structural constraints. The research spans multiple contexts—from linear to nonlinear elasticity, from local boundary control to contact conditions, and from classical variational formulations to modern phase-field and gradient flow methods—demonstrating both theoretical depth and practical relevance.

In Chapter 2, we investigated the optimal control problem in linear elasticity, where the objective is to match a target displacement field through the use of boundary control. This chapter incorporates frictional contact boundary conditions and employs a combined approach using topological derivatives and level-set methods to evolve and optimize the structural shape. The analysis also includes a preliminary discussion of the turnpike property in optimal control problems.

Chapter 3 shifts focus to the detailed analysis of contact problems, where a phase-field method is adopted to represent potential contact interfaces smoothly. This approach avoids the numerical challenges posed by traditional inequality-based models. Furthermore, the chapter investigates topology optimization under phase-field modeling, illustrating how contact mechanics and geometric shape design are coupled through variational principles and numerical simulations.

In Chapter 4, we explore the gradient flow theory in the context of shape optimization with PDE constraints. Emphasis is placed on constructing energy-dissipation-based shape evolution models, which lead to gradient flows governed by partial differential equations. Numerical examples confirm the effectiveness of this method in driving shape updates while respecting mechanical constraints.

Chapter 5 extends the framework to nonlinear elasticity, particularly under large deformation scenarios. To address the limitations of conventional finite element methods in capturing complex geometries, we employ a discontinuous Galerkin (DG) method

combined with level-set techniques for shape evolution. This approach exhibits strong adaptability and stability when dealing with nonlinear material behavior and moving boundaries.

Future Research Directions

Based on the current work, several promising directions are identified for future investigation:

- Rigorous analysis and extension of the turnpike property: While the turnpike behavior was preliminarily addressed in this thesis, its applicability to elasticity systems, nonlinear systems, time-dependent boundaries, and multiphysics settings remains to be rigorously established and numerically tested.
- Integration of phase-field methods with multiscale modeling: Extending the phase-field framework to multiscale designs—for example, in microstructured or functionally graded materials—would enable finer control of mechanical performance and structural functionality.
- Learning-based guidance in topology optimization: Incorporating machine learning, especially deep neural networks, to guide the evolution of level sets or topological derivatives could enhance convergence rates and global search capabilities.
- Gradient flow analysis in nonlinear and dynamic settings: While the current gradient flow formulations are mainly applicable to steady-state and linear problems, extending them to nonlinear materials and dynamic systems presents both theoretical and computational challenges.
- Efficient numerical algorithms for contact problems: Given the computational cost of variational inequality and phase-field formulations for contact, developing efficient solvers, such as adaptive meshing, parallel computing, or multilevel methods, is a vital future direction.

Code

Code for the Contact problem

This FreeFEM++ program solves a three-dimensional linear elastic problem with frictional contact using the regularized Tresca friction model. The geometry and computational mesh are created using the widely used open source mesh generation tool Gmsh and then imported into FreeFEM++ as a tetrahedral mesh. The computational domain contains different boundary regions labeled as Dirichlet (fixed displacement), Neumann (applied loads), and contact (potential friction interaction).

The material behavior is governed by a standard linear isotropic elastic model characterized by Young's modulus and Poisson's ratio. Contact along the specified surfaces is treated using a Tresca-type friction law that imposes an upper limit on the tangential contact stress. For numerical differentiation and stability, the Tresca friction condition is regularized using a smooth approximation of the tangential norm.

The resulting nonlinear variational problem is solved using Newton's method. At each iteration, the code assembles and solves a linearized problem using the FreeFEM++ "problem" structure. The solution is updated incrementally and convergence is checked via the L^2 norm of the displacement increments. The normal vectors on the contact boundaries are accessible via "N.x", "N.y" and "N.z" and are used to extract the tangential components required for the friction formulation.

After convergence, the computed displacement field is exported in ".vtu" format for post-processing and visualization, e.g. using ParaView. This implementation demonstrates how to use regularization techniques and Newton-type solvers in the FreeFEM++ framework, supported by the external mesh generation capabilities of Gmsh, to efficiently solve complex nonlinear friction contact problems.

```
// 3D Tresca Frictional Contact Problem with Regularization
//using Newton's Method in FreeFEM++ (problem-form + iteration)
```

```

// Material parameters
real E = 1;
real nu = 0.3;
real lambda = E*nu/((1+nu)*(1-2*nu));
real mu = E/(2*(1+nu));

// Contact and regularization parameters
real sigmatr = 10;
real eta = 1e-3;
real fz = -10;

// Define function space
fespace Vh(Th, [P2, P2, P2]);
Vh [u1, u2, u3], [v1, v2, v3];

// Newton iteration parameters
real tol = 1e-8;
int maxIter = 30;
int iter = 0;
real resNorm = 1e5;

// Temporary variables to track update
Vh [du1, du2, du3];

while ((resNorm > tol) && (iter < maxIter)) {
    iter++;

    problem TrescaContact([du1, du2, du3], [v1, v2, v3]) =
        int3d(Th)(
            lambda*(dx(du1)+dy(du2)+dz(du3))*(dx(v1)+dy(v2)+dz(v3))
            + 2*mu*(
                dx(du1)*dx(v1) + dy(du2)*dy(v2) + dz(du3)*dz(v3)
                + (dy(du1)+dx(du2))*(dy(v1)+dx(v2))/2
                + (dz(du1)+dx(du3))*(dz(v1)+dx(v3))/2
            )
        )
}

```

```

        + (dz(du2)+dy(du3))*(dz(v2)+dy(v3))/2
    )
)
+ int2d(Th, Contact)(
    sigmatr * (
        (
            (u1 - (u1*N.x + u2*N.y + u3*N.z)*N.x)
            * (v1 - (v1*N.x + v2*N.y + v3*N.z)*N.x)
            + (u2 - (u1*N.x + u2*N.y + u3*N.z)*N.y)
            * (v2 - (v1*N.x + v2*N.y + v3*N.z)*N.y)
            + (u3 - (u1*N.x + u2*N.y + u3*N.z)*N.z)
            * (v3 - (v1*N.x + v2*N.y + v3*N.z)*N.z)
        )
        /
        max(sqrt(
            sqr(u1 - (u1*N.x + u2*N.y + u3*N.z)*N.x)
            + sqr(u2 - (u1*N.x + u2*N.y + u3*N.z)*N.y)
            + sqr(u3 - (u1*N.x + u2*N.y + u3*N.z)*N.z)
        ), eta)
    )
)
- int3d(Th)( 0*v1 + 0*v2 + fz*v3 )
- int2d(Th, Applied)( 0*v1 + 0*v2 + fz*v3 )
+ on(Dirichlet, du1=0, du2=0, du3=0);

TrescaContact;

// Update solution
u1[] += du1[];
u2[] += du2[];
u3[] += du3[];

resNorm = sqrt(du1[].12 + du2[].12 + du3[].12);
cout << "[Newton] Iteration " << iter
<< ", Residual Norm = " << resNorm << endl;

```

}

This program implements a phase-field-based structural optimization framework using the Allen–Cahn gradient flow equation. The optimization is carried out in a three-dimensional domain discretized using a tetrahedral mesh, which is generated externally using Gmsh and imported into FreeFEM++.

The phase-field variable φ represents the material distribution, where $\varphi \approx 1$ corresponds to solid material and $\varphi \approx -1$ to void. The evolution of φ is driven by the minimization of a total energy functional that combines elastic compliance (via pre-computed strain energy density) and interfacial regularization (based on a double-well potential).

The Allen–Cahn model is chosen for its simplicity and computational efficiency. It formulates the time-dependent evolution of the phase field as an L^2 -gradient descent of the energy functional. A semi-implicit time-stepping scheme is used: the nonlinear double-well potential is treated explicitly, while the curvature term (involving the Laplacian of φ) is handled implicitly for numerical stability.

In each time step, the following sequence is performed:

- Solve for the auxiliary variable $\beta_\epsilon = W'(\varphi) - \epsilon^2 \Delta \varphi$,
- Compute the chemical potential μ , which includes both the elastic and regularization contributions,
- Update the phase field φ by solving the semi-implicit Allen–Cahn equation.

The implementation uses FreeFEM++ macros for efficient expression of nonlinear potential derivatives and material interpolation. The output phase-field variable is exported in VTK format for post-processing and visualization.

```
// Phase Field Optimization
//using Allen-Cahn Gradient Flow in FreeFEM++

real eps = 0.01;
real gamma = 1.0;
real etaTilde = 1.0;
real dt = 0.01;
int nSteps = 100;
```

```

// Finite element space
fespace Vh(Th, P1);
Vh phi, phiOld, beta, mu, muel, test;

// Double-well potential W and derivatives
macro W1(x) (2.0 * (x) * ((x)*(x) - 1.0)) // W'(phi)
macro W2(x) (6.0 * (x)*(x) - 2.0) // W''(phi)

// Time-stepping loop
for (int n = 0; n < nSteps; n++) {

    // STEP 1: Solve for beta
    varf vBeta(betaTemp, test) =
        int3d(Th)( betaTemp * test )
    - int3d(Th)( W1(phiOld) * test )
    - int3d(Th)( eps^2 * ( dx(phi) * dx(test)
        + dy(phi) * dy(test) + dz(phi) * dz(test) ) );
    matrix Mbeta = vBeta(Vh, Vh);
    set(Mbeta, solver=CG);
    beta[] = Mbeta^-1 * 0;

    // STEP 2: Compute mu = mu_el + etaTilde * mu_ph
    muel[] = 0;
    for (int i = 0; i < phi.ndof; i++) {
        muel[][i] = 0.5 * chiPrime(phi[][i]) * A1minusA0 * strainEnergy[][i];
    }

    mu = muel + etaTilde * (
        - (1.0 / eps) * (dx(dx(beta)) + dy(dy(beta)) + dz(dz(beta)))
        + ( (1.0 / eps^3) * W2(phiOld) + gamma / (2 * eps) ) * beta
    );

    // STEP 3: Update phi using semi-implicit Allen-Cahn step
    varf vPhi(phiTemp, test) =
        int3d(Th)( (phiTemp - phiOld) / dt * test + mu * test );

```

```

matrix Mphi = vPhi(Vh, Vh);
set(Mphi, solver=CG);
phi[] = Mphi^-1 * 0;

phiOld = phi;
cout << "Step " << n << " completed.\n";
}

// Export result
savevtk("phiFinal.vtu", Th, phi, dataname="phasefield");

```

Code for the Gradient Flow

In this first part of the code using python, we define the physical and numerical parameters for a shape optimization problem set in a two-dimensional annular region—that is, the area between two concentric circles with radii r_{inner} and r_{outer} . The simulation aims to evolve a deformable internal boundary (interface) within this annulus to minimize a PDE-constrained objective function.

The domain is discretized in polar coordinates. The angular coordinate θ is divided into N_{theta} equally spaced points, representing the resolution of the circular interface. For each angular direction, the radial direction is discretized into two segments: N_{r1} points from the inner boundary to the interface, and N_{r2} points from the interface to the outer boundary.

Material properties are defined via the diffusion coefficients $a1$ and $a2$, which apply to the subregions separated by the moving interface. The outer boundary condition values for two PDEs are set using G (Dirichlet condition) and F_{flux} (Neumann flux). The evolution of the interface is governed by a gradient flow method, controlled by a small time step dt and a regularization weight $epsilon$.

To initialize the shape of the internal interface, a function $init_r$ is defined. It constructs a perturbed circle by adding a finite number of sinusoidal modes (Fourier components) to a base radius $a0$. The coefficients for the cosine and sine modes are randomly sampled within a small range using a_{coeffs} and b_{coeffs} , introducing small-scale irregularities. This results in a closed curve $r(\theta)$ that is smooth but not perfectly circular. The interface is then clipped to ensure it stays safely within the domain

boundaries, avoiding the inner and outer edges by a small *margin*.

```
# -----
# parameters
# -----
r_inner, r_outer = 0.3, 2.0
margin = 1e-3
N_theta, N_r1, N_r2 = 60, 15, 15
a1, a2 = 2.0, 1.0
G, F_flux = 2.5902671654458267, 1.0
epsilon = 0.1
dt = 1e-3
num_steps = 500
np.random.seed(42)
N_modes = 8
a0 = 1.2
a_coeffs = np.random.uniform(-0.05, 0.05, N_modes)
b_coeffs = np.random.uniform(-0.05, 0.05, N_modes)
theta = np.linspace(0, 2*np.pi, N_theta, endpoint=False)

def init_r(theta):
    r = a0 * np.ones_like(theta)
    for n in range(1, N_modes+1):
        r += a_coeffs[n-1]*np.cos(n*theta) + b_coeffs[n-1]*np.sin(n*theta)
    return np.clip(r, r_inner+margin, r_outer-margin)

def compute_geometry(fx, fy, theta):
    dtheta = theta[1] - theta[0]
    d_fx = (np.roll(fx,-1) - np.roll(fx,1)) / (2*dtheta)
    d_fy = (np.roll(fy,-1) - np.roll(fy,1)) / (2*dtheta)
    metric = d_fx**2 + d_fy**2
    tau_x = d_fx/np.sqrt(metric); tau_y = d_fy/np.sqrt(metric)
    nx, ny = -tau_y, tau_x

    d2_fx = (np.roll(fx,-1) - 2*fx + np.roll(fx,1)) / (dtheta**2)
    d2_fy = (np.roll(fy,-1) - 2*fy + np.roll(fy,1)) / (dtheta**2)
```

```

kappa = (d_fx*d2_fy - d_fy*d2_fx) / (metric1.5)
kx, ky = kappa*nx, kappa*ny

ds = np.sqrt(metric)*dtheta
dkx_ds = (np.roll(kx,-1) - np.roll(kx,1)) / (2*ds)
dky_ds = (np.roll(ky,-1) - np.roll(ky,1)) / (2*ds)
d2kx_ds2 = (np.roll(dkx_ds,-1) - np.roll(dkx_ds,1)) / (2*ds)
d2ky_ds2 = (np.roll(dky_ds,-1) - np.roll(dky_ds,1)) / (2*ds)

return nx, ny, kappa, kx, ky, d2kx_ds2, d2ky_ds2

def assemble_system(points, tri, is_inner):
    n = points.shape[0]
    K = lil_matrix((n,n))
    F = np.zeros(n)
    for idx, elm in enumerate(tri.simplices):
        V = points[elm]
        area = 0.5 * np.linalg.det(np.hstack((np.ones((3,1)), V)))
        b = np.array([V[(i+1)%3,1] - V[(i+2)%3,1] for i in range(3)])
        c = np.array([V[(i+2)%3,0] - V[(i+1)%3,0] for i in range(3)])
        a = a1 if is_inner[idx] else a2
        Ke = (a/(4*area)) * (np.outer(b,b) + np.outer(c,c))
        for i_loc,I in enumerate(elm):
            for j_loc,J in enumerate(elm):
                K[I,J] += Ke[i_loc,j_loc]
    return K, F

r_int = init_r(theta)
snapshots = [(0, r_int.copy())]

```

This part represents the core loop of the simulation, where the interface shape evolves over a sequence of time steps. At each iteration, the current interface shape $r_{int}(\theta)$ is used to build a polar mesh over the domain. For each angular direction θ , radial points are sampled from the inner boundary to the interface (N_{r1} points), and then from the interface to the outer boundary (N_{r2} points). These points are collected in Cartesian coordinates, forming a point cloud representing the geometry of the current

annular domain sliced by the interface.

Once the mesh points are generated, Delaunay triangulation is applied to construct a valid triangulated mesh, which is essential for solving partial differential equations (PDEs) using the finite element method (FEM). The triangles are then classified into two types: “inner” and “outer” elements, depending on whether their centroids fall inside or outside the current interface $r_{int}(\theta)$. This classification allows us to assign different material properties ($a1$ or $a2$) to each triangle.

Two PDEs are solved in each time step. The first PDE solves for a scalar field w using Dirichlet boundary conditions: it is set to zero on the inner boundary and to a constant G on the outer boundary. The second PDE solves for a different scalar field u , this time using a Neumann boundary condition (flux F_{flux}) on the outer boundary and zero Dirichlet on the inner boundary. These two fields model physical quantities like temperature or potential, under different types of external control.

To solve these PDEs, the stiffness matrix K and the load vector F are assembled for the current mesh using linear basis functions. Boundary conditions are enforced directly in the matrix system by overwriting rows for constrained nodes. Finally, both PDEs are solved using a sparse linear solver (*spsolve*), yielding the numerical solutions w and u over the entire mesh for this iteration.

This entire process prepares the data needed to compute how the interface should evolve in the next steps, by measuring how well the current shape satisfies the optimization goal.

```

fx = r_int*np.cos(theta); fy = r_int*np.sin(theta)
nx, ny, kappa, kx, ky, kss_x, kss_y = compute_geometry(fx, fy, theta)
pts=[]; iface_idx=[]
for j,t in enumerate(theta):
    radial = np.hstack((
        np.linspace(r_inner, r_int[j], N_r1),
        np.linspace(r_int[j], r_outer, N_r2)
    ))
    base=len(pts)
    for k,rr in enumerate(radial):
        pts.append((rr*np.cos(t), rr*np.sin(t)))
        if k==N_r1-1:
            iface_idx.append(base+k)
pts = np.array(pts)

```

```

pts_u, idx_u, inv = np.unique(pts, axis=0,
                               return_index=True, return_inverse=True)

points = pts_u
node_ids = [inv[i] for i in iface_idxxs]
tri = Delaunay(points)
cent = points[tri.simplices].mean(axis=1)
thetac = np.mod(np.arctan2(cent[:,1], cent[:,0]),2*np.pi)
rc = np.linalg.norm(cent,axis=1)
iface_r = np.interp(thetac,theta,r_int)
is_inner = rc <= iface_r

#PDE
K1,F1 = assemble_system(points,tri,is_inner)
dists = np.linalg.norm(points,axis=1)
bc_in = dists<=r_inner+1e-6
bc_out = dists>=r_outer-1e-6
for i in np.where(bc_in|bc_out)[0]:
    K1[i,:]=0; K1[i,i]=1; F1[i]=0 if bc_in[i] else G
w = spsolve(csr_matrix(K1),F1)

K2,F2 = assemble_system(points,tri,is_inner)
for i in np.where(bc_in)[0]:
    K2[i,:]=0; K2[i,i]=1; F2[i]=0
edges=set()
for elm in tri.simplices:
    for k in range(3):
        p,q=elm[k],elm[(k+1)%3]
        if (abs(np.linalg.norm(points[p])-r_outer)<1e-6 and
            abs(np.linalg.norm(points[q])-r_outer)<1e-6):
            edges.add(tuple(sorted((p,q))))
for i,j in edges:
    L=np.linalg.norm(points[i]-points[j])
    F2[i]+=F_flux*L/2; F2[j]+=F_flux*L/2
K2=csr_matrix(K2); K2.setdiag(K2.diagonal()+1e-8)
u = spsolve(K2,F2)

```

After obtaining the numerical solutions w and u from the PDEs, the code proceeds to compute the shape derivative—that is, the gradient of the objective function with respect to the shape of the interface. This is the critical step that determines how the interface should evolve to reduce the cost functional.

First, the gradients ∇w and ∇u are computed element-wise over the mesh using standard FEM gradient evaluation within each triangle. These gradients are then averaged over nodes within the inner and outer regions separately, yielding smoothed approximations of ∇w and ∇u on both sides of the interface. This averaging is weighted by element area to ensure consistency.

Next, for each interface node, the normal component of the gradient is computed on both sides of the interface using the pre-computed unit normal vectors (nx, ny) . The differences in these normal derivatives across the interface (so-called jump terms) are essential for determining how much the PDE solutions are affected by small perturbations in the interface. Two main quantities are formed: the jump in $\frac{\partial w}{\partial n}$ and the jump in $\frac{\partial u}{\partial n}$, both of which feed into the shape derivative of the cost functional.

The resulting scalar field dJ_{scalar} represents, for each angular direction θ , how the objective function would change if the interface moved slightly outward or inward in that direction. This field serves as a gradient descent direction. To ensure smoothness and prevent the formation of sharp or unstable shapes, a curvature-based regularization term is added. This term penalizes high curvature and promotes smoother interface evolution, analogous to mean curvature flow.

The interface is then updated by moving each point along the direction defined by the combined velocity Vn , which consists of both the negative shape derivative and the regularization term scaled by a small constant *epsilon*. Since the interface is parameterized radially, this velocity is projected onto the radial direction at each θ before applying the update. The result is a new interface shape $r_{int(\theta)}$ for the next time step, which is then clipped to ensure it remains within the valid annular domain.

This gradient-based update mechanism is the optimization engine of the code—it drives the interface toward shapes that reduce the PDE mismatch between u and w .

```
n_pts=points.shape[0]
gw_in=np.zeros((n_pts,2)); gw_out=np.zeros((n_pts,2))
gu_in=np.zeros((n_pts,2)); gu_out=np.zeros((n_pts,2))
area_in=np.zeros(n_pts); area_out=np.zeros(n_pts)
for idx,elm in enumerate(tri.simplices):
    V=points[elm]
```

```

area=0.5*np.linalg.det(np.hstack((np.ones((3,1)),V)))
b=np.array([V[(i+1)%3,1]-V[(i+2)%3,1] for i in range(3)])
c=np.array([V[(i+2)%3,0]-V[(i+1)%3,0] for i in range(3)])
gradN=np.vstack((b,c))/(2*area)
gw_e=gradN.dot(w[elm]); gu_e=gradN.dot(u[elm])
if is_inner[idx]:
    for I in elm:
        gw_in[I]+=gw_e*area; gu_in[I]+=gu_e*area; area_in[I]+=area
else:
    for I in elm:
        gw_out[I]+=gw_e*area; gu_out[I]+=gu_e*area; area_out[I]+=area

gw_in_safe = np.zeros_like(gw_in)
gu_in_safe = np.zeros_like(gu_in)
gw_out_safe = np.zeros_like(gw_out)
gu_out_safe = np.zeros_like(gu_out)
mask_in = area_in > 1e-12
mask_out = area_out > 1e-12
gw_in_safe[mask_in] = gw_in[mask_in] / area_in[mask_in, None]
gu_in_safe[mask_in] = gu_in[mask_in] / area_in[mask_in, None]
gw_out_safe[mask_out] = gw_out[mask_out] / area_out[mask_out, None]
gu_out_safe[mask_out] = gu_out[mask_out] / area_out[mask_out, None]
normals = np.stack((nx,ny),axis=1)
dn_w_in = (gw_in_safe[node_ids]*normals).sum(axis=1)
dn_w_out = (gw_out_safe[node_ids]*normals).sum(axis=1)
dn_u_in = (gu_in_safe[node_ids]*normals).sum(axis=1)
dn_u_out = (gu_out_safe[node_ids]*normals).sum(axis=1)
jump_dn_w=dn_w_in-dn_w_out; jump_dn_u=dn_u_in-dn_u_out
term_u=(a1*dn_u_in - a2*dn_u_out)*jump_dn_u
term_w=(a1*dn_w_in - a2*dn_w_out)*jump_dn_w
part1=2*(term_u-term_w)
nu_in=np.sum(gu_in_safe[node_ids]2,axis=1)
nu_out=np.sum(gu_out_safe[node_ids]2,axis=1)
nw_in=np.sum(gw_in_safe[node_ids]2,axis=1)
nw_out=np.sum(gw_out_safe[node_ids]2,axis=1)

```

```

part2=(a1*nu_in - a2*nu_out) - (a1*nw_in - a2*nw_out)
dJ_scalar = part1 - part2

# 8) Update
curv_reg = ((kss_x + 0.5*kappa2*nx - kx)*nx +
            (kss_y + 0.5*kappa2*ny - ky)*ny)
Vn = -epsilon*curv_reg - dJ_scalar
e_r_dot_n = nx*np.cos(theta) + ny*np.sin(theta)
dr = dt * Vn * e_r_dot_n
r_int += dr
r_int = np.clip(r_int, r_inner+margin, r_outer-margin)

```

This final part of the code is responsible for monitoring and visualizing the shape optimization process over time. Every 50 time steps, the algorithm evaluates the objective functional J , which quantifies the discrepancy between the two PDE solutions w and u . Specifically, it calculates the integrated energy of the difference in their gradients, weighted by the corresponding material coefficient ($a1$ or $a2$) over the entire domain. This provides a scalar value that indicates how well the current interface configuration satisfies the optimization goal: minimizing the gradient mismatch.

At each of these checkpoints, the current shape of the interface $r_{int}(\theta)$ is stored in the *snapshots* list along with the step number. This allows the algorithm to record the history of interface shapes, enabling post-process analysis or visual presentation of the optimization trajectory.

Once the time-stepping loop concludes, the code generates a multi-panel plot showing snapshots of the interface at different stages. For each stored shape, it reconstructs the full polar mesh, re-triangulates it, and overlays the interface curve on top of the mesh. The triangulation is shaded in a neutral color to provide spatial context, while the evolving interface is plotted in red to highlight how its geometry changes over time.

```

if snapshots[-1][0] != num_steps:
    snapshots.append((num_steps, r_int.copy()))

n_snap = len(snapshots)
cols = 4
rows = int(np.ceil(n_snap / cols))
fig, axes = plt.subplots(rows, cols, figsize=(4 * cols, 4 * rows))
axes = axes.flatten()

```

```

for ax, (st, r_snap) in zip(axes, snapshots):
    fx = r_snap * np.cos(theta)
    fy = r_snap * np.sin(theta)
    pts = []
    for j, t in enumerate(theta):
        radial = np.hstack((
            np.linspace(r_inner, r_snap[j], N_r1),
            np.linspace(r_snap[j], r_outer, N_r2)
        ))
        for rr in radial:
            pts.append((rr * np.cos(t), rr * np.sin(t)))
    pts = np.unique(np.array(pts), axis=0)
    tri_snap = Delaunay(pts)
    cent_snap = pts[tri_snap.simplices].mean(axis=1)
    mask = np.linalg.norm(cent_snap, axis=1) >= r_inner + 1e-6

    ax.triplot(pts[:, 0], pts[:, 1], tri_snap.simplices[mask],
               color='lightgray', lw=0.5)
    fx_c = np.hstack([fx, fx[0]])
    fy_c = np.hstack([fy, fy[0]])
    ax.plot(fx_c, fy_c, 'r-', lw=2)
    ax.set_title(f"Step {st}")
    ax.set_aspect('equal')
    ax.set_xticks([]);
    ax.set_yticks([])

for ax in axes[n_snap:]:
    ax.axis('off')

plt.tight_layout()
plt.show()

```

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Acknowledgements

Acknowledgements

As I approach the conclusion of my doctoral studies in Poland, I reflect upon this academic journey with a profound sense of gratitude. My experience studying in Poland has undoubtedly been one of the most enriching, invaluable, and transformative chapters of my life. This cross-border pursuit of knowledge not only broadened my academic horizons but also deeply shaped my character and mindset. From the initial confusion and unease upon entering a foreign land to gradually adapting to a new environment, rooting myself in scholarly work, and expanding my research domain, the entire process has been both challenging and rewarding—a journey of growth and transformation.

At the outset, the unfamiliar language, cultural context, and academic system left me feeling disoriented. However, through continuous adaptation and exploration, I gradually found my direction. With the meticulous guidance of my supervisor and the support and encouragement of my peers, I developed the ability to conduct independent research and delved into the field of shape and topology optimization. This journey not only honed my professional competence but also cultivated resilience and a proactive spirit.

I am deeply fortunate to have had the opportunity to live and study in Poland—a country steeped in history and brimming with modern vitality. Here, I gained access to a wealth of academic resources and experienced a rigorous research environment. I was equally enriched by the multicultural atmosphere that fostered inclusiveness and diversity. Whether through the daily routine of scholarly inquiry, the stimulating exchanges at academic conferences, or the small moments of everyday life on Polish streets, these experiences have become indelible memories. I am especially grateful that I am now able to submit my doctoral dissertation, a testament to and culmination of this extraordinary experience.

I wish to extend my sincerest gratitude and highest respect to my Polish super-

visor, Professor Jan Sokołowski. His unwavering support, insightful guidance, and extraordinary patience enabled me to make steady progress in my research. His encouragement and trust continuously motivated me to move forward with confidence and enthusiasm, face challenges courageously, and strive toward academic excellence. As an internationally renowned expert in the field of shape and topology optimization, it has been a great honor to be his doctoral student and to benefit from his mentorship.

Throughout the doctoral process, Professor Sokołowski demonstrated exceptional dedication and a strong sense of responsibility. Whenever I encountered difficulties in my research, he would patiently address my questions, often explaining concepts multiple times until I fully understood them. His guidance was remarkably thorough—every idea, every derivation was meticulously recorded in his notebooks and personally handed to me, which greatly enriched my understanding. His rigorous and patient approach to scholarship taught me not only how to solve academic problems but also instilled in me a deeper appreciation for the spirit and attitude of scientific research.

Despite his demanding schedule, Professor Sokołowski consistently made time for weekly face-to-face meetings. Even when he was traveling on official duties, we maintained regular academic communication through online platforms without interruption. His commitment to his students and his professional integrity are truly admirable. Through him, I came to realize that true academic mentorship lies not only in the transmission of knowledge but also in the guidance of spirit.

Professor Sokołowski also gave me great support in academic exchanges. He attached great importance to my growth in the international academic arena and actively encouraged me to participate in various academic activities. One of the most memorable experiences was that I was invited to give a 45-minute lecture at the Department of Mathematics of Jagiellonian University on his recommendation. Giving a lecture at this world-renowned and long-established university was my first international lecture in my life, which was a milestone for me. In addition, with his encouragement and recommendation, I also gave academic reports at international conferences such as the 28th International Conference on Methods and Models in Automation and Robotics (MMAR 2024) and the 95th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM 2025). These valuable experiences have greatly improved my scientific research expression ability and international communication level, and also allowed me to have a deeper understanding of the significance and value of international academic cooperation.

On a personal level, Professor Sokołowski was kind, approachable, and generous

with his support. He frequently invited me to share coffee and desserts, guided me in exploring the historical and cultural landscape of Warsaw, and engaged in rich conversations beyond academic topics. His passion for nature, music, and history—alongside his breadth of knowledge and intellectual charm—earned my deepest admiration.

I am also profoundly grateful to my Chinese advisor, Professor Shengfeng Zhu, who has played a pivotal role throughout my academic development. He has been both a mentor and a trusted guide since my early academic journey. From the start of my master's program, Professor Zhu provided patient and enthusiastic supervision. At a time when my research ideas were immature and my direction unclear, he offered timely and effective guidance. His rigorous academic standards, sharp research instincts, and ability to convey complex concepts with clarity helped me establish a solid foundation in scientific methodology and inquiry. His uncompromising pursuit of academic excellence has left a lasting impact on me.

In particular, Professor Zhu's support during the critical phase of preparing for my studies abroad was instrumental. He thoughtfully mapped out an academic trajectory for me, introduced me to Professor Sokołowski, and assisted me in preparing application documents and reference letters. His help laid the groundwork for my successful transition to the international academic community. After I arrived in Poland, Professor Zhu consistently followed my research progress, regularly engaged with me on academic issues, and provided professional guidance and advice. On a personal level, he provided generous financial assistance during my doctoral studies, alleviating my practical concerns and enabling me to focus wholeheartedly on research.

During my time in Poland, Professor Zhu also made an academic visit to the country and met with me in Warsaw for in-depth discussions on my research topics. He offered valuable suggestions and insights for my doctoral dissertation, which played a crucial role in shaping and refining the direction of my research.

I would also like to express heartfelt thanks to Professor Sokołowski's wife for her kindness and support during my stay in Poland. Her generosity and attentiveness contributed significantly to my well-being and gave me a sense of warmth and respect far from home.

Special thanks go to Meizhi Qian, whose companionship made my initial experience in Poland far less daunting. Her presence brought me comfort and reassurance during a time of great transition. She provided immense support in every aspect of my adjustment to a new country—academically, linguistically, culturally, and personally. Whether it was navigating unfamiliar academic expectations, overcoming language bar-

riers, understanding local customs, or simply managing daily life, she was always there to offer guidance and encouragement. Her generosity, care, and unwavering companionship were invaluable to me, and I am deeply grateful for everything she has done to ease my journey and help me feel at home in a foreign land.

I would also like to extend my sincere thanks to all colleagues and friends at the Institute of the Polish Academy of Sciences. Your camaraderie and support brought joy and vitality to my daily life. In particular, I thank Chang Gao, Shengjie Li, Yunxiang Lu, Zhuoxuan Li, Bruck Gio, and Tran Hung. Each of you contributed to making this journey fulfilling and memorable. I will always cherish the time we spent together.

My heartfelt gratitude also goes to my roommate Zixuan Zhang, whose companionship has been a source of comfort and support. Her presence gave me a sense of home away from home during challenging moments.

Most importantly, I am deeply indebted to my parents for their unconditional love, understanding, and unwavering support. They have always stood behind me, enabling me to persevere and reach this point. I also thank my younger siblings, whose encouragement and trust have never waned despite the great distance between us. You are the source of my strength and a constant reminder of the importance and warmth of family.

With my deepest appreciation,

Yixin Tan

Warszawa, Poland, June